

March 1994

LSENS, A General Chemical Kinetics and Sensitivity Analysis Code for Homogeneous Gas-Phase Reactions

III. Illustrative Test Problems

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Preface

LSENS, the Lewis General Chemical Kinetics and Sensitivity Analysis Code, has been developed for homogeneous, gas-phase chemical kinetics computations and contains sensitivity analysis for a variety of problems, including nonisothermal situations. The code is described in a series of three reference publications, which also provide a detailed guide to its use and many illustrative test problems.

LSENS has been designed for accuracy, efficiency, flexibility, and convenience. A variety of chemical reaction models can be considered: static system; steady, one-dimensional, inviscid flow; reaction behind an incident shock wave, including boundary layer correction; and perfectly stirred (highly backmixed) reactor. In addition, the chemical equilibrium state can be computed for the assigned states of temperature and pressure, enthalpy and pressure, temperature and volume, and internal energy and volume. Any reaction problem can be adiabatic, have an assigned heat transfer profile, or for static and flow problems, have an assigned-temperature profile. For static problems either the density is constant or the pressure-versus-time profile is assigned. For flow problems either the pressure or area can be assigned as a function of time or distance. For a static reaction sensitivity coefficients of the dependent variables and their temporal derivatives with respect to the initial values of the dependent variables and/or the three rate coefficient parameters of the chemical reactions can be obtained.

LSENS checks the legality and sufficiency of all input. At the user's option LSENS checks the reaction mechanism for uniqueness and ensures that each reaction satisfies charge and atom balance requirements.

Part I of the series (NASA RP-1328), consisting of chapters 1 to 7, presents the theory and the numerical solution procedures used in LSENS. The ordinary differential equations (ODE's) describing chemical kinetics problems are derived in chapter 2. Chapter 3 describes the numerical integration method and how it is implemented. In chapter 4 the governing ODE's for sensitivity analysis are derived and the solution method and numerical algorithm explained. The governing equations and solution methods for the chemical equilibrium state, equilibrium and frozen thermodynamic states behind an incident shock wave, and perfectly stirred reactor problems are presented in chapters 5 to 7.

Part II of the series (NASA RP-1329), consisting of chapters 8 to 13 and appendixes A to C, describes LSENS, its usage, and how to modify it. Chapter 8 describes the computational capabilities and convenience features built into the code. Chapter 9 presents its structure and description. Chapter 10 lists modifications that may be required to implement LSENS on the user's computer system. Chapter 11 provides a guide to code usage and describes how to prepare the input data files required to execute LSENS. The output information generated by the code is discussed in chapter 12. Example problems illustrating both problem data file construction and code usage are given in chapter 13. These examples supplement chapter 11 by providing additional guidance on preparation of the problem data file.

Preface

The partial derivatives required by the numerical solution procedures detailed in chapters 3, 4, and 7 are derived in appendix A. Appendix B shows how to access the system clock for several common computing systems so that execution times can be measured. Appendix C describes the modifications required to change the built-in values for various quantities.

This volume, part III of the series (appendixes D and E), explains the example problems provided with LSENS and presents sample results. Appendix D describes the kinetics test cases. These problems illustrate the various reaction models that can be solved by, and options built into, LSENS. Appendix E describes the kinetics-plus-sensitivity-analysis test cases supplied with the code. The examples in the two appendixes cover a variety of problem types and so should serve as useful models for the structure of the problem data file required to execute the code. Indeed, it is likely that the desired file can be produced by modifying one of the test cases.

Details regarding code availability and procurement can be obtained from COSMIC, 328 East Broad Street, University of Georgia, Athens, GA 30602 (Telephone: 706-542-3265).

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Appendix D

Kinetics Test Cases

In this appendix we describe 16 kinetics-only (i.e., no sensitivity analysis) test cases that are provided with the code. These cases were chosen to illustrate both the problem types that can be solved by LSENS and the options built into it. Therefore users can find among them a model problem that can be easily modified to suit their needs. In order to demonstrate the various options for the ACTION switch, all cases were set up in a single data file, which is listed in table D.1. We now describe each problem in some detail, including the source of the chemical mechanism used.

Description of Test Cases

Case 1

The first case illustrates the shock-wave-initiated adiabatic decomposition of pure bromine. It shows the use of the shock kinetics option and the boundary layer correction for area given by Mirels (refs. 1 to 3). The variable SHOCK is set to TRUE in namelist PROB and the boundary layer parameters LSUBM and ETA are also given. The values of pressure, Mach number, and temperature in namelist START are the incident shock conditions. The inert species xenon is listed on the line following the blank line that signals the end of the reaction list. The composition of the initial (unshocked) gas mixture is given as mole fractions following namelist START, and the list is ended with an END line. The rate expression used for the decomposition reaction was measured by Warshay (ref. 4). The namelist SOLVER, which lists the error control parameters EMAX and ATOLSP, is at the end of the data, just before the FINIS card, which ends the case.

Case 2

Test case 2 is a stoichiometric hydrogen-air ignition in supersonic flow through a constant-area duct with heat transfer from the system computed as a linear function of tem-

perature. For this and all other completely new cases the word NEW appears on the ACTION line after the title. The hydrogen-oxygen reaction mechanism is that of Brabbs and Musiak (ref. 5), and the nitrogen-oxygen-hydrogen reactions are from Brabbs et al. (ref. 6). Namelist PROB contains the area profile information (the constant area CX0), the heat transfer equation coefficients HT0 and HT1, and the list of print stations (in centimeters) in the array PRINT. Initial composition is given by the special input, which specifies fuel name and stoichiometry plus equivalence ratio for the fuel-standard air mixture in namelist START. The fuel name, H2, appears in columns 41 and 42 of the integration and assigned variables, units, and fuel name line. Because the standard air contains small percentages of nonreacting carbon dioxide and argon, these species are listed as inert species after the reaction list.

Case 3

This third case is the same problem as case 2 and illustrates the use of the CHANGE and ADD options of the ACTION switch. We have temporarily changed the pre-exponential factor for the reaction $2\text{HO}_2 \rightleftharpoons \text{H}_2\text{O}_2 + \text{O}_2$ and added the reaction of an oxygen atom with H_2O_2 to the mechanism to test the effect of these changes on the computed results. Both the CHANGE and ADD lists end with a blank line. The word REPEAT should not be used after the ADD list because LSENS automatically uses the rest of the mechanism and other data that are unchanged from the previous case. On the integration and assigned variables, units, and fuel name line U.S. customary (FPS) units have been specified for the input of any new data. The only new information that is given in namelist PROB is the print station list (in feet). We have also set the variable EXCHR equal to TRUE to obtain the printout of net energy exchange rates for each reaction instead of the net reaction conversion rates. In namelist START initial temperature and pressure are given in U.S. customary units, and the mass fuel-oxidant ratio is given for the initial mixture. The stoichiometric coefficients of the

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fuel are not needed when this ratio is given, but they are saved automatically when the ADD or REPEAT option is used. Comparing the computed results of cases 2 and 3 showed close agreement. Therefore the two changes made in the mechanism for this case were not used in any other test cases.

Case 4

Case 4 is the ignition of a stoichiometric hydrogen-oxygen mixture flowing in a duct whose pressure profile is assigned as a linear function of distance. The flow is subsonic and heat transfer is assigned as a linear function of temperature. The default value of QMREAD is TRUE; it has been set in namelist PROB only for illustrative purposes. The chemical mechanism is the hydrogen-oxygen portion of the mechanism of case 2, and the initial composition is given by the same method used for that case. However, because the oxidant is pure oxygen rather than the standard air, the variables ARAT, NOXRAT, and CRAT are set equal to zero. Output is specified in U.S. customary (FPS) units, but input is in the default (CGS) units. Therefore, the values given in the array PRINT are in centimeters.

Case 5

Case 5 is the static ignition of a methane-oxygen-nitrogen mixture with an assigned pressure profile that increases linearly with time. Heat transfer from the system is given by the Otto cycle correlation option in LSENS. Note that in namelist PROB the logical variable QMREAD must now be set equal to FALSE, and values of the variables BORE, STROKE, TWALL, and RPM are given. The chemical mechanism builds on that of case 2 by adding the oxidation and decomposition reactions of methane and its oxidation products ethane, ethylene, and acetylene, as well as the reactions of carbon monoxide and the formyl (HCO) radical. Also included are reactions of ketene (C_2H_2O), the ketyl (C_2HO) radical, and formaldehyde. All C-H-O reactions were taken from references 7 and 8. Initial mixture composition is given by listing species mole fractions after namelist START.

Case 6

Case 6 is the adiabatic ignition of a methane-oxygen-nitrogen mixture in supersonic flow at a constant assigned pressure of 1.73 atm. A trace amount of CN radical is also present in the oxidant. The chemical mechanism is the same as for case 5. In namelist PROB the logical variable COMBUS has been set equal to TRUE so that the code will perform an assigned-pressure and assigned-enthalpy equilibrium computation, which gives the final conditions that the kinetics computations would approach at long reaction times.

With the pressure assigned, LSENS computes a reaction area profile as a function of distance.

Case 7

Case 7 is the same methane-air problem as case 6. However, the area profile computed in case 6 is now assigned as a table of distance and area values, and pressure is computed. We illustrate here the use of the REPEAT option of the ACTION switch. Output is requested at values of the area that are listed in the array APRINT, and COMBUS is set equal to FALSE so that an equilibrium calculation is not performed. Computed results are close to, but not identical to, those of case 6. Small differences arise because area is now computed by interpolation from the table of values at each step.

Case 8

Case 8 is also the same methane-air problem as case 6. Now both the area and temperature profiles computed in case 6 are assigned as tables of values. The REPEAT option is used again to save data from the previous case, including the area-versus-distance table that was used in case 7. Because temperature is assigned as a function of distance in namelist TMPDAT, output is requested at values of temperature, which are assigned in the array TPRINT. Note that only pressure and Mach number are assigned in namelist START.

Case 9

Case 9 is a methane-air reaction in supersonic flow with both temperature and pressure assigned constant values. The REPEAT option is used again so that the chemical mechanism of case 6 is used. The variable COMBUS is set equal to TRUE so that an assigned-pressure and assigned-temperature equilibrium problem will be performed before the kinetic computation. Note that the constant pressure is assigned by setting CX0 in namelist PROB and the assigned constant temperature is given by setting CX0 in namelist TMPDAT.

Case 10

Case 10 is the adiabatic, constant-volume ignition of methanol and oxygen in a static system. The mechanism was obtained by adding to the reactions of case 6 ten reactions involving methanol and CH_2OH taken from reference 9. The variable RHOCON is set equal to TRUE in namelist PROB. The simplified combustion input is used for this rich (fuel-oxygen equivalence ratio, 2.0) mixture. However, very small initial concentrations of three trace species are also read in following namelist START. These additional mole fractions may be read in if their sum does not exceed the code error limit (1.0×10^{-4}) for the deviation of the initial mole fraction

sum from unity. Note also that the starting pressure of 1 atm is written as 760 mm of mercury and the variable MMHG is set equal to TRUE in namelist START.

Case 11

Case 11 illustrates a propane-air perfectly stirred reactor (PSR) combustion process followed by a flow reaction of the products expanding through a diverging nozzle. The reaction mechanism is obtained by adding three propane and propyl radical reactions (ref. 8) to the methane-air mechanism of case 6. We demonstrate, first of all, a typical assigned-mass-flow-rate PSR problem setup in namelist WSPROB and, second, the option to perform an assigned-area flow problem by using the output conditions from the PSR as input conditions for the flow problem. The variables WELSTR and WSFLOW have both been set equal to TRUE in namelist PROB. However, setting only WSFLOW equal to TRUE also tells LSENS to set WELSTR equal to TRUE and perform both problems. Note that the data for the flow problem in namelist PROB include the setting of the logical variable ROCKET equal to TRUE for rocket performance parameter computations. Values of ATHROT and PC must also be given.

Case 12

Case 12 is the high-temperature ionization of air in constant-area subsonic flow. It shows the use of the logical variables DBUGO and ORDER in namelist PROB to obtain the individual net molar formation rates of each species by every reaction in which the species participates. Setting ORDER equal to TRUE is probably more useful, because the net production rates are printed in order of decreasing magnitude and none of the zero rates are printed. The chemical mechanism contains reactions of both neutral and ionic species. Rate expressions for neutral-species reactions are the same as those used for previous test cases. However, the conversion between oxygen atoms and molecular oxygen is written as the recombination process here. The rate expression for it is taken from reference 10, with the preexponential factor increased because the collision partners are N_2 and O_2 instead of argon. Rate expressions for ion-molecule reactions were taken from reference 11.

Case 13

Case 13 is the high-pressure reaction of hydrogen and carbon monoxide in a constant-volume, constant-temperature static system. The variable COMBUS is set equal to TRUE to obtain an assigned-temperature and assigned-volume equilibrium computation. The variables RHOCON and TCON are set equal to TRUE in namelist PROB, and initial tempera-

ture and pressure are assigned in namelist START. The chemical mechanism is a small portion of the mechanism of case 6.

Case 14

Case 14 is the photolytic ignition of a stoichiometric hydrogen-oxygen mixture in a constant-volume static system. The variable COMBUS is set equal to TRUE to obtain an assigned-internal-energy and assigned-volume equilibrium computation. The chemical mechanism is that of case 4 with the addition of the photolysis of the H_2 and O_2 molecules. The constant rate coefficients for these reactions were set arbitrarily to give ignition at about 1 s of reaction time.

Case 15

Case 15 is a methane-air ignition reaction in supersonic flow with the area profile assigned as a table of monotonically decreasing values in the array ATB as a function of the increasing XTB values (namelist PROB). The print stations are assigned at values of the area and are given in the array APRINT. Note that they are given in decreasing order, as are the ATB values, and that values different from those in the area table may be given. The first value in the ATB array should not be given in the APRINT array. It will be ignored if present. For this problem initial values of temperature, Mach number, and pressure are set in namelist START.

Case 16

Case 16 is the same as case 15 except for the designation of print stations, and therefore the REPEAT action option has been used. The print stations are listed as values of distance in the array PRINT and are, of course, in increasing order. We have repeated the ATB and XTB arrays in namelist PROB for illustration purposes only. These arrays are saved by use of the REPEAT option and do not have to be listed again unless the user wants to do so.

Listing of Results

The test case file in table D.1 was executed on a Sun SPARCstation 1 computer using the Sun 4.1.3 operating system and the Sun FORTRAN compiler using level 2 optimization except for subroutine KINP, which had to be compiled with no optimization. Sample pages from the output are shown in table D.2. The total execution time for all 16 test cases was approximately 154 s. This time will be significantly shorter for mainframe computers and the current more powerful workstations from Sun and other manufacturers.

TABLE D.1.—PROBLEM DATA FILE FOR KINETICS-ONLY TEST CASES

```

TAPE
  LSENS   BROMINE DISSOCIATION IN A SHOCK TUBE
  M       + BR2       =2.0BR
  THIRDBODY
BR2       3.80      END

XE
DISTANCE AREA
  &prob lsubm=32200.0, eta=0.5, shock=.true.,
  print=0.05,2.0,4.0, &end
  &start p=0.1227, mach=3.2646, t=299.9, &end
BR2       0.01
XE        0.99
END
&solver emax=1.0E-2, atolsp=1.0E-10, &end
FINIS
  LSENS   HYDROGEN - AIR TEST WITH HEAT TRANSFER
  NEW
    O      + H2O      = OH      + OH      6.8E+13  0.      18365.
    H      + O2       = OH      + O       1.89E+14  0.      16400.
    O      + H2       = OH      + H       4.20E+14  0.      13750.
    H      + HO2      = H2      + O2      7.28E+13  0.      2126.
    O      + HO2      = OH      + O2      5.0E+13  0.      1000.
    HO2    + OH       = H2O     + O2      8.0E+12  0.      0.
    H      + HO2      =2.0OH    + O2      1.34E+14  0.      1070.
    H2     + HO2      = H2O2    + H       7.91E+13  0.      25000.
    OH     + H2O2     = H2O     + HO2     6.1E+12  0.      1430.
    HO2    + HO2      = H2O2    + O2      1.8E+12  0.      0.
    H      + H2O2     = OH      + H2O     7.8E+11  0.      0.
    M      + H2O2     =2.0OH    + H2O     1.44E+17  0.      45510.
  THIRDBODY
H2        2.30      O2        .78      H2O      6.0      H2O2      6.6
END
    H2     + OH       = H2O     + H       4.74E+13  0.      6098.
    H      + O2       = HO2     + M       1.46E+15  0.      -1000.
  THIRDBODY
O2        1.30      N2        1.3      H2O      21.3      H2        3.0
END
    M      + H2O      = H       + OH      1.30E+15  0.      105140.
  THIRDBODY
H2        4.00      O2        1.5      H2O      20.0      N2        1.5
END
    H      + O        = OH      + M       7.1E+18  -1.      0.
    M      + H2       = H       + H       2.2E+14  0.      96000.
  THIRDBODY
H2        4.10      O2        2.0      H2O      15.0      N2        2.0
END
    M      + O2       = O       + O       1.80E+18  -1.      118020.
    HO2    + NO       = NO2     + OH      2.09E+12  0.      -477.
    O      + NO2      = NO      + O2      1.0E+13  0.      596.
    NO     + O        = NO2     + M       5.62E+15  0.      -1160.
    NO2    + H        = NO      + OH      3.47E+14  0.      1470.
    NO     + O        = N       + O2      3.8E+9   1.      41370.
    O      + N2       = NO      + N       1.8E+14  0.      76250.
    NO     + H        = N       + OH      2.63E+14  0.      50410.
    M      + N2O      = N2      + O       6.92E+23  -2.5    65000.
    O      + N2O      = N2      + O2      1.0E+14  0.      28020.
    O      + N2O      =2.0NO    + O2      6.92E+13  0.      26630.
    N      + NO2      =2.0NO    + O2      4.0E+12  0.      0.
    N2O    + H        = N2      + OH      7.59E+13  0.      15100.
    NO2    + H2       = HNO2    + H       2.4E+13  0.      29000.
    OH     + NO2      = HNO3    + M       3.0E+15  0.      -3800.
  THIRDBODY
O2        0.70      H2        1.4      END
    OH     + NO       = HNO2    + M       5.6E+15  0.      -1700.
    HNO    + H        = H2      + NO      5.0E+12  0.      0.
    H      + NO       = HNO     + M       5.4E+15  0.      -600.
    HNO    + OH       = H2O     + NO      3.6E+13  0.      0.

CO2       AR
DISTANCE AREA
  &prob cx0=2000.0, print=3.048,6.096,7.620,12.19,
  htran=.true., qmread=.true., htl=5.863, ht0=-42.88, &end
  &start p=0.956, t=1559.0, mach=5.0,
  eratio=1.0, scc=0.0, sch=2.0, scox=0.0, &end
END
&solver emax=5.0E-3, atolsp=1.0E-12, &end
FINIS
  LSENS   HYDROGEN - AIR TEST WITH HEAT TRANSFER
  FULL MECHANISM
  CASE 3

```

TABLE D.1.—Continued.

```

CHANGE
HO2      +   HO2      =   H2O2      +   O2              2.0E+12  0.      0.

ADD
O        +   H2O2      =   OH        +   HO2              8.0E+13  0.      1000.

END
DISTANCE AREA      FPS      H2
&prob exchr=.true., print=0.1,0.2,0.25,0.4, &end
&start p=2023.09, t=2806.2, mach=5.0,
      flair=0.029163, &end
END
&solver &end
FINIS
LSSENS   HYDROGEN - OXYGEN CASE WITH HEAT TRANSFER
NEW
O        +   H2O      =   OH        +   OH              6.8E+13  0.      18365.
H        +   O2       =   OH        +   O               1.89E+14  0.      16400.
O        +   H2       =   OH        +   H              4.20E+14  0.      13750.
H        +   HO2      =   H2        +   O2              7.28E+13  0.      2126.
O        +   HO2      =   OH        +   O2              5.0E+13  0.      1000.
HO2      +   OH       =   H2O      +   O2              8.0E+12  0.      0.
H        +   HO2      =2.0OH      +   O               1.34E+14  0.      1070.
H2       +   HO2      =   H2O2     +   H              7.91E+13  0.      25000.
OH       +   H2O2     =   H2O      +   HO2             6.1E+12  0.      1430.
HO2      +   HO2      =   H2O2     +   O2              1.8E+12  0.      0.
H        +   H2O2     =   OH        +   H2O             7.8E+11  0.      0.
M        +   H2O2     =2.0OH      +   O               1.44E+17  0.      45510.
THIRDBODY
H2       2.30      O2              .78      H2O              6.0      H2O2      6.6
END
H2       +   OH       =   H2O      +   H              4.74E+13  0.      6098.
H        +   O2       =   HO2      +   M              1.46E+15  0.      -1000.
THIRDBODY
O2       1.30      H2              3.0      H2O              21.3      END
M        +   H2O      =   H        +   OH              1.30E+15  0.      105140.
THIRDBODY
H2       4.00      O2              1.5      H2O              20.0      END
H        +   O        =   OH        +   M              7.1E+18  -1.      0.
M        +   H2       =   H        +   H              2.2E+14  0.      96000.
THIRDBODY
H2       4.10      O2              2.0      H2O              15.0      END
M        +   O2       =   O        +   O              1.80E+18  -1.      118020.

END
DISTANCE PRESSURE      FPS      H2
&prob cx0=5.0, cx1=.01, print=10.0,15.0,15.95,
      htran=.true., qmread=.true., ht1=5.863, ht0=-42.88, &end
&start t=1050.0, mach=0.5, area=2000.0, eratio=1.0,
      scc=0.0, sch=2.0, scox=0.0, noxrat=0.0, arat=0.0, crat=0.0, &end
END
&solver emax=5.0E-6, atolsp=1.0E-13, &end
FINIS
LSSENS   CH4 - O2 - N2 MECH. BATCH RXN. WITH OTTO CYCLE HEAT LOSS
NEW
M        +   CH4      =   CH3      +   H              2.0E+17  0.      88000.
H        +   CH4      =   CH3      +   H2             1.26E+14  0.      11900.
CH4      +   O2       =   CH3      +   HO2             7.94E+13  0.      56000.
O        +   CH4      =   CH3      +   OH              1.9E+14  0.      11720.
OH       +   CH4      =   CH3      +   H2O             2.5E+13  0.      5010.
CH3      +   O2       =   CH3O     +   O               2.4E+13  0.      28680.
CH3      +   OH       =   CH3O     +   H               6.3E+12  0.      0.
M        +   CH3O     =   CH2O     +   H               5.0E+13  0.      21000.
CH3      +   CH3      =   C2H6     +   H               2.4E+14  -.4    0.
H        +   C2H6     =   C2H5     +   H2             1.32E+14  0.      9700.
O        +   C2H6     =   C2H5     +   OH              1.13E+14  0.      7850.
OH       +   C2H6     =   C2H5     +   H2O             8.7E+13  0.      3520.
M        +   C2H5     =   C2H4     +   H               1.0E+17  0.      31000.
C2H5     +   O2       =   C2H4     +   HO2             2.0E+12  0.      5000.
H        +   C2H5     =   C2H4     +   H2              4.8E+13  0.      0.
CH3      +   CH2      =   C2H4     +   H               2.0E+13  0.      0.
H        +   C2H4     =   H2       +   C2H3            1.5E+14  0.      10200.
M        +   C2H4     =   C2H2     +   H2              2.6E+17  0.      79300.
C2H4     +   OH       =   C2H3     +   H2O             4.8E+12  0.      1230.
C2H4     +   OH       =   CH3      +   CH2O             2.0E+12  0.      960.
C2H4     +   O        =   CH3      +   HCO             3.3E+12  0.      1130.
C2H4     +   O        =   CH2O     +   CH2             2.5E+13  0.      5000.
M        +   C2H3     =   C2H2     +   H               3.0E+15  0.      32000.
C2H3     +   O2       =   CH2O     +   HCO             3.98E+12  0.      -250.
C2H3     +   H        =   C2H2     +   H2              6.0E+12  0.      0.
C2H3     +   O        =   C2H2O    +   H               3.3E+13  0.      0.
C2H3     +   OH       =   C2H2     +   H2O             5.0E+12  0.      0.

```

TABLE D.1.—Continued.

C2H3	+	CH2	=	C2H2	+	CH3	3.0E+13	0.	0.
C2H3	+	C2H	=	2.0C2H2			3.0E+13	0.	0.
M	+	C2H2	=	C2H	+	H	4.2E+16	0.	107000.
C2H2	+	O	=	CH2	+	CO	1.6E+14	.0	9890.
C2H2	+	O	=	C2HO	+	H	4.0E+14	0.0	10660.
C2H2	+	OH	=	C2H	+	H2O	6.3E+12	0.0	7000.
C2H2	+	OH	=	C2H2O	+	H	3.2E+11	0.0	200.
C2H	+	O2	=	C2HO	+	O	5.00E+13	0.	1500.
C2H	+	OH	=	C2HO	+	H	2.0E+13	0.	0.
C2HO	+	O2	=	2.0CO	+	OH	1.46E+12	0.	2500.
C2HO	+	O	=	2.0CO	+	H	1.202E+12	0.	0.
C2HO	+	OH	=	2.0HCO			1.0E+13	0.	0.
C2HO	+	H	=	CH2	+	CO	5.0E+13	0.	0.
C2HO	+	CH2	=	C2H3	+	CO	3.0E+13	0.	0.
C2HO	+	CH2	=	CH2O	+	C2H	1.0E+13	0.	2000.
	2.0C2H2O		=	C2H2	+	2.0CO	1.0E+13	0.	0.
C2H2O	+	OH	=	CH2O	+	HCO	2.8E+13	0.	0.
C2H2O	+	OH	=	C2HO	+	H2O	7.5E+12	0.	3000.
C2H2O	+	H	=	CH3	+	CO	1.13E+13	0.	3428.
C2H2O	+	H	=	C2HO	+	H2	7.5E+13	0.	8000.
C2H2O	+	O	=	C2HO	+	OH	5.0E+13	0.	8000.
C2H2O	+	O	=	CH2O	+	CO	2.0E+13	0.	0.
M	+	C2H2O	=	CH2	+	CO	2.0E+16	0.	60000.
C2H	+	O	=	CO	+	CH	5.0E+13	0.	0.
CH3O	+	O2	=	CH2O	+	HO2	1.0E+13	0.	7170.
CH3O	+	H	=	CH2O	+	H2	2.0E+13	0.	0.
M	+	CH2O	=	HCO	+	H	5.0E+16	0.	81000.
CH2O	+	OH	=	HCO	+	H2O	3.0E+13	0.	1200.
CH2O	+	H	=	HCO	+	H2	2.5E+13	0.	3990.
CH2O	+	O	=	HCO	+	OH	3.5E+13	0.	3500.
CH3	+	CH2O	=	CH4	+	HCO	1.0E+10	0.5	6000.
CH3	+	HCO	=	CH4	+	CO	3.0E+11	.5	0.
CH3	+	HO2	=	CH3O	+	OH	2.0E+13	0.	0.
M	+	CH3	=	CH2	+	H	1.95E+16	0.	91600.
H	+	CH3	=	H2	+	CH2	2.7E+11	.67	25700.
O	+	CH3	=	OH	+	CH2	1.9E+11	.68	25700.
OH	+	CH3	=	H2O	+	CH2	2.7E+11	.67	25700.
CH	+	CO2	=	HCO	+	CO	3.7E+12	0.	0.
CH	+	O2	=	HCO	+	O	1.0E+13	0.	0.
CH2	+	O2	=	CH2O	+	O	5.0E+11	0.5	6960.
CH2	+	O	=	CH	+	OH	2.0E+11	.7	25800.
CH2	+	OH	=	CH	+	H2O	5.0E+11	.5	5900.
CH2	+	H	=	CH	+	H2	3.2E+11	0.7	4970.
CH2	+	CH2	=	C2H3	+	H	5.0E+12	0.	0.
CH2	+	CH2	=	C2H2	+	H2	4.0E+13	0.	0.
HCO	+	O2	=	CO	+	HO2	3.0E+13	0.	0.
HCO	+	O	=	CO	+	OH	3.0E+13	0.	0.
HCO	+	OH	=	CO	+	H2O	3.0E+13	0.	0.
HCO	+	H	=	CO	+	H2	2.0E+13	0.	0.
M	+	HCO	=	H	+	CO	2.9E+14	0.	15570.
CO	+	O	=	CO2	+	M	2.4E+15	0.	4100.
CO	+	O2	=	CO2	+	O	2.5E+12	0.	47690.
CO	+	OH	=	CO2	+	H	4.17E+11	0.	1000.
CO	+	HO2	=	CO2	+	OH	5.75E+13	0.	22930.
O	+	H2O	=	OH	+	OH	6.8E+13	0.	18365.
H	+	O2	=	OH	+	O	1.89E+14	0.	16400.
O	+	H2	=	OH	+	H	4.20E+14	0.	13750.
H	+	HO2	=	H2	+	O2	7.28E+13	0.	2126.
O	+	HO2	=	OH	+	O2	5.0E+13	0.	1000.
HO2	+	OH	=	H2O	+	O2	8.0E+12	0.	0.
H	+	HO2	=	2.0OH			1.34E+14	0.	1070.
H2	+	HO2	=	H2O2	+	H	7.91E+13	0.	25000.
OH	+	H2O2	=	H2O	+	HO2	6.1E+12	0.	1430.
HO2	+	HO2	=	H2O2	+	O2	1.8E+12	0.	0.
H	+	H2O2	=	OH	+	H2O	7.8E+11	0.	0.
M	+	H2O2	=	2.0OH			1.44E+17	0.	45510.
THIRDBODY									
H2	2.30	O2		.78	H2O	6.0	H2O2	6.6	
END									
H2	+	OH	=	H2O	+	H	4.74E+13	0.	6098.
H	+	O2	=	HO2	+	M	1.46E+15	0.	-1000.
THIRDBODY									
O2	1.30	N2		1.3	H2O	21.3	CO2	7.0	
END									
M	+	H2O	=	H	+	OH	1.30E+15	0.	105140.
THIRDBODY									
H2	4.00	O2		1.5	H2O	20.0	N2	1.5	
CO2	4.0	END							
H	+	O	=	OH	+	M	7.1E+18	-1.	0.
M	+	H2	=	H	+	H	2.2E+14	0.	96000.
THIRDBODY									
H2	4.10	O2		2.0	H2O	15.0	N2	2.0	

TABLE D.1.—Continued.

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END
M      + O2      = O      + O      1.80E+18  -1.    118020.
CH     + N2      = HCN     + N      1.0E+11   0.     19000.
CN     + H2      = HCN     + H      6.0E+13   0.     5300.
O      + HCN     = OH      + CN      1.4E+11   .68    16900.
OH     + HCN     = HNCO    + H      4.0E+11   0.     2800.
CN     + O       = CO      + N      1.2E+13   0.     0.
CN     + OH      = NCO     + H      2.5E+14   0.     6000.
H2     + NCO     = HNCO    + H      1.0E+14   0.     9000.
HNCO   + H       = NH2     + CO      1.0E+14   0.     8500.
CN     + O2      = NCO     + O      3.2E+13   0.     1000.
CN     + CO2     = NCO     + CO      3.7E+12   0.     0.
O      + NCO     = NO      + CO      2.0E+13   0.     0.
N      + NCO     = N2      + CO      1.0E+13   0.     0.
H      + NCO     = NH      + CO      2.0E+13   0.     0.
CH     + NO      = N       + HCO     1.6E+13   0.     9940.
CH     + NO      = O       + HCN     2.0E+12   0.     0.
NH     + OH      = N       + H2O     5.0E+11   0.5    2000.
HO2    + NO      = NO2     + OH      2.09E+12  0.     -477.
O      + NO2     = NO      + O2      1.0E+13   0.     596.
NO     + O       = NO2     + M       5.62E+15  0.     -1160.
NO2    + H       = NO      + OH      3.47E+14  0.     1470.
NO     + H       = N       + OH      2.63E+14  0.     50410.
NO     + O       = N       + O2      3.8E+9    1.     41370.
O      + N2      = NO      + N      1.80E+14  0.     76250.
N      + NO2     =2.O NO    4.0E+12   0.     0.
M      + N2O     = N2      + O      6.92E+23  -2.5    65000.
O      + N2O     = N2      + O2      1.0E+14   0.     28020.
O      + N2O     =2.O NO    6.92E+13  0.     26630.
N2O    + H       = N2      + OH      7.59E+13  0.     15100.
NO2    + H2      = HNO2    + H      2.4E+13   0.     29000.
OH     + NO2     = HNO3    + M      3.0E+15   0.     -3800.
THIRDBODY
O2     0.70      H2     1.4      END
OH     + NO      = HNO2    + M      5.6E+15  0.     -1700.
HNO    + H       = H2      + NO      5.0E+12   0.     0.
H      + NO      = HNO     + M      5.4E+15  0.     -600.
HNO    + OH      = H2O     + NO      3.6E+13   0.     0.

END
TIME      PRESSURE
&prob ct0=2.0, cti=700.0, print=2.5E-4,3.4E-4,3.8E-4,
      htran=.true., qmread=.false., otto=.true., bore=8.5, stroke=7.0,
      twall=1000.0, rpm=2500.0, &end
&start t=1550.0, &end
CH4     0.1725
O2      0.1725
N2      0.65492
N       0.00001
CH      0.00003
CN      0.00001
CH2     0.00001
END
&solver emax=1.0E-4, atolsp=1.0E-13, &end
FINIS
LSSENS  METHANE  AIR    MECHANISM  CONSTANT PRESSURE FLOW PROBLEM  CASE 6
NEW
M      + CH4     = CH3     + H      2.0E+17  0.     88000.
H      + CH4     = CH3     + H2     1.26E+14  0.     11900.
CH4    + O2      = CH3     + HO2    7.94E+13  0.     56000.
O      + CH4     = CH3     + OH      1.9E+14  0.     11720.
OH     + CH4     = CH3     + H2O     2.5E+13  0.     5010.
CH3    + O2      = CH3O    + O      2.4E+13  0.     28680.
CH3    + OH      = CH3O    + H      6.3E+12  0.     0.
M      + CH3O    = CH2O    + H      5.0E+13  0.     21000.
CH3    + CH3     = C2H6    - .4    0.
H      + C2H6    = C2H5    + H2     1.32E+14  0.     9700.
O      + C2H6    = C2H5    + OH     1.13E+14  0.     7850.
OH     + C2H6    = C2H5    + H2O     8.7E+13  0.     3520.
M      + C2H5    = C2H4    + H      1.0E+17  0.     31000.
C2H5   + O2      = C2H4    + HO2    2.0E+12  0.     5000.
H      + C2H5    = C2H4    + H2     4.8E+13  0.     0.
CH3    + CH2     = C2H4    + H      2.0E+13  0.     0.
H      + C2H4    = H2      + C2H3  1.5E+14  0.     10200.
M      + C2H4    = C2H2    + H2     2.6E+17  0.     79300.
C2H4   + OH      = C2H3    + H2O     4.8E+12  0.     1230.
C2H4   + OH      = CH3     + CH2O    2.0E+12  0.     960.
C2H4   + O       = CH3     + HCO     3.3E+12  0.     1130.
C2H4   + O       = CH2O    + CH2     2.5E+13  0.     5000.
M      + C2H3    = C2H2    + H      3.0E+15  0.     32000.
C2H3   + O2      = CH2O    + HCO     3.98E+12  0.     -250.
C2H3   + H       = C2H2    + H2     6.0E+12  0.     0.

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TABLE D.1.—Continued.

C2H3	+	O	=	C2H2O	+	H	3.3E+13	0.	0.
C2H3	+	OH	=	C2H2	+	H2O	5.0E+12	0.	0.
C2H3	+	CH2	=	C2H2	+	CH3	3.0E+13	0.	0.
C2H3	+	C2H	=	2.0C2H2			3.0E+13	0.	0.
M	+	C2H2	=	C2H	+	H	4.2E+16	0.	107000.
C2H2	+	O	=	CH2	+	CO	1.6E+14	.0	9890.
C2H2	+	O	=	C2HO	+	H	4.0E+14	0.0	10660.
C2H2	+	OH	=	C2H	+	H2O	6.3E+12	0.0	7000.
C2H2	+	OH	=	C2H2O	+	H	3.2E+11	0.0	200.
C2H	+	O2	=	C2HO	+	O	5.00E+13	0.	1500.
C2H	+	OH	=	C2HO	+	H	2.0E+13	0.	0.
C2HO	+	O2	=	2.0CO	+	OH	1.46E+12	0.	2500.
C2HO	+	O	=	2.0CO	+	H	1.202E+12	0.	0.
C2HO	+	OH	=	2.0HCO			1.0E+13	0.	0.
C2HO	+	H	=	CH2	+	CO	5.0E+13	0.	0.
C2HO	+	CH2	=	C2H3	+	CO	3.0E+13	0.	0.
C2HO	+	CH2	=	CH2O	+	C2H	1.0E+13	0.	2000.
		2.0C2HO	=	C2H2	+	2.0CO	1.0E+13	0.	0.
C2H2O	+	OH	=	CH2O	+	HCO	2.8E+13	0.	0.
C2H2O	+	OH	=	C2HO	+	H2O	7.5E+12	0.	3000.
C2H2O	+	H	=	CH3	+	CO	1.13E+13	0.	3428.
C2H2O	+	H	=	C2HO	+	H2	7.5E+13	0.	8000.
C2H2O	+	O	=	C2HO	+	OH	5.0E+13	0.	8000.
C2H2O	+	O	=	CH2O	+	CO	2.0E+13	0.	0.
M	+	C2H2O	=	CH2	+	CO	2.0E+16	0.	60000.
C2H	+	O	=	CO	+	CH	5.0E+13	0.	0.
CH3O	+	O2	=	CH2O	+	HO2	1.0E+13	0.	7170.
CH3O	+	H	=	CH2O	+	H2	2.0E+13	0.	0.
M	+	CH2O	=	HCO	+	H	5.0E+16	0.	81000.
CH2O	+	OH	=	HCO	+	H2O	3.0E+13	0.	1200.
CH2O	+	H	=	HCO	+	H2	2.5E+13	0.	3990.
CH2O	+	O	=	HCO	+	OH	3.5E+13	0.	3510.
CH3	+	CH2O	=	CH4	+	HCO	1.0E+10	0.5	6000.
CH3	+	HCO	=	CH4	+	CO	3.0E+11	.5	0.
CH3	+	HO2	=	CH3O	+	OH	2.0E+13	0.	0.
M	+	CH3	=	CH2	+	H	1.95E+16	0.	91600.
H	+	CH3	=	H2	+	CH2	2.7E+11	.67	25700.
O	+	CH3	=	OH	+	CH2	1.9E+11	.68	25700.
OH	+	CH3	=	H2O	+	CH2	2.7E+11	.67	25700.
CH	+	CO2	=	HCO	+	CO	3.7E+12	0.	0.
CH	+	O2	=	HCO	+	O	1.0E+13	0.	0.
CH2	+	O2	=	CH2O	+	O	5.0E+11	0.5	6960.
CH2	+	O	=	CH	+	OH	2.0E+11	.7	25800.
CH2	+	OH	=	CH	+	H2O	5.0E+11	.5	5900.
CH2	+	H	=	CH	+	H2	3.2E+11	0.7	4970.
CH2	+	CH2	=	C2H3	+	H	5.0E+12	0.	0.
CH2	+	CH2	=	C2H2	+	H2	4.0E+13	0.	0.
HCO	+	O2	=	CO	+	HO2	3.0E+13	0.	0.
HCO	+	O	=	CO	+	OH	3.0E+13	0.	0.
HCO	+	OH	=	CO	+	H2O	3.0E+13	0.	0.
HCO	+	H	=	CO	+	H2	2.0E+13	0.	0.
M	+	HCO	=	H	+	CO	2.9E+14	0.	15570.
CO	+	O	=	CO2	+	M	2.4E+15	0.	4100.
CO	+	O2	=	CO2	+	O	2.5E+12	0.	47690.
CO	+	OH	=	CO2	+	H	4.17E+11	0.	1000.
CO	+	HO2	=	CO2	+	OH	5.75E+13	0.	22930.
O	+	H2O	=	OH	+	OH	6.8E+13	0.	18365.
H	+	O2	=	OH	+	O	1.89E+14	0.	16400.
O	+	H2	=	OH	+	H	4.20E+14	0.	13750.
H	+	HO2	=	H2	+	O2	7.28E+13	0.	2126.
O	+	HO2	=	OH	+	O2	5.0E+13	0.	1000.
HO2	+	OH	=	H2O	+	O2	8.0E+12	0.	0.
H	+	HO2	=	2.0OH			1.34E+14	0.	1070.
H2	+	HO2	=	H2O2	+	H	7.91E+13	0.	25000.
OH	+	H2O2	=	H2O	+	HO2	6.1E+12	0.	1430.
HO2	+	HO2	=	H2O2	+	O2	1.8E+12	0.	0.
H	+	H2O2	=	OH	+	H2O	7.8E+11	0.	0.
M	+	H2O2	=	2.0OH			1.44E+17	0.	45510.
THIRDBODY									
H2		2.30	O2		.78	H2O	6.0	H2O2	6.6
END									
H2	+	OH	=	H2O	+	H	4.74E+13	0.	6098.
H	+	O2	=	HO2	+	M	1.46E+15	0.	-1000.
THIRDBODY									
O2		1.30	N2		1.3	H2O	21.3	CO2	7.0
END									
M	+	H2O	=	H	+	OH	1.30E+15	0.	105140.
THIRDBODY									
H2		4.00	O2		1.5	H2O	20.0	N2	1.5
CO2		4.0	END						
H	+	O	=	OH	+	M	7.1E+18	-1.	0.
M	+	H2	=	H	+	H	2.2E+14	0.	96000.

TABLE D.1.—Continued.

H2	THIRDBODY	4.10	O2	2.0	H2O	15.0	N2	2.0
END								
M	+	O2	=	O	+	O	1.80E+18	-1.
CH	+	N2	=	HCN	+	N	1.0E+11	0.
CN	+	H2	=	HCN	+	H	6.0E+13	0.
O	+	HCN	=	OH	+	CN	1.4E+11	.68
OH	+	HCN	=	HNCO	+	H	4.0E+11	0.
CN	+	O	=	CO	+	N	1.2E+13	0.
CN	+	OH	=	NCO	+	H	2.5E+14	0.
H2	+	NCO	=	HNCO	+	H	1.0E+14	0.
HNCO	+	H	=	NH2	+	CO	1.0E+14	0.
CN	+	O2	=	NCO	+	O	3.2E+13	0.
CN	+	CO2	=	NCO	+	CO	3.7E+12	0.
O	+	NCO	=	NO	+	CO	2.0E+13	0.
N	+	NCO	=	N2	+	CO	1.0E+13	0.
H	+	NCO	=	NH	+	CO	2.0E+13	0.
CH	+	NO	=	N	+	HCO	1.6E+13	0.
CH	+	NO	=	O	+	HCN	2.0E+12	0.
NH	+	OH	=	N	+	H2O	5.0E+11	0.5
HO2	+	NO	=	NO2	+	OH	2.09E+12	0.
O	+	NO2	=	NO	+	O2	1.0E+13	0.
NO	+	O	=	NO2	+	M	5.62E+15	0.
NO2	+	H	=	NO	+	OH	3.47E+14	0.
NO	+	H	=	N	+	OH	2.63E+14	0.
NO	+	O	=	N	+	O2	3.8E+9	1.
O	+	N2	=	NO	+	N	1.80E+14	0.
N	+	NO2	=	2.0NO			4.0E+12	0.
M	+	N2O	=	N2	+	O	6.92E+23	-2.5
O	+	N2O	=	N2	+	O2	1.0E+14	0.
O	+	N2O	=	2.0NO			6.92E+13	0.
N2O	+	H	=	N2	+	OH	7.59E+13	0.
NO2	+	H2	=	HNO2	+	H	2.4E+13	0.
OH	+	NO2	=	HNO3	+	M	3.0E+15	0.
THIRDBODY								
O2		0.70	H2	1.4	END			
OH	+	NO	=	HNO2	+	M	5.6E+15	0.
HNO	+	H	=	H2	+	NO	5.0E+12	0.
H	+	NO	=	HNO	+	M	5.4E+15	0.
HNO	+	OH	=	H2O	+	NO	3.6E+13	0.

END

DISTANCE PRESSURE

```

&prob cx0=1.730, combus=.true., exchr=.true.,
  print=10.0,20.0,25.0,30.0,32.0,34.0,36.0,37.0,38.0,39.0,40.0,41.0,
    42.0,43.0,44.0,45.0,46.0,47.0,48.0, &end
&start area=1000.0, mach=2.0, t=1700.0, &end
CH4      0.049768
O2       0.199072
N2       0.75116
CN       0.0000001
END

```

```

&solver emax=1.0E-4, atolsp=1.0E-10, &end

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FINIS

LENS METHANE - AIR WITH AREA PROFILE OF CASE 6

CASE 7

REPEAT

DISTANCE AREA

```

&prob pcon=.false., combus=.false.,
  xtb=0.0,10.0,20.0,25.0,30.0,32.0,34.0,36.0,37.0,38.0,39.0,40.0,41.0,
    42.0,43.0,44.0,45.0,46.0,47.0,48.0,
  atb= 1000.00,1000.20,1004.65,1010.85,1023.22,1031.44,1042.92,1059.73,
    1071.45,1087.06,1110.03,1153.75,1284.24,1350.79,1376.81,1397.15,
    1414.00,1428.05,1439.83,1449.81,
  aprint=1023.22,1153.75,1439.83, &end
&start t=1700.0, mach=2.0, p=1.730, &end
CH4      0.049768
O2       0.199072
N2       0.75116
CN       0.0000001
END

```

```

&solver emax=5.0E-5, atolsp=1.0E-13, &end

```

FINIS

LENS METHANE - AIR WITH AREA AND TEMPERATURE PROFILES OF CASE 6

CASE 8

REPEAT

DISTANCE AREA

```

&prob tass=.true., &end
&ttmpdat xtb=0.0,15.0,20.0,25.0,30.0,32.0,34.0,36.0,38.0,40.0,41.0,
    42.0,43.0,44.0,45.0,46.0,47.0,48.0,
  ttmpb=1700.00,1702.50,1707.74,1718.03,1738.22,1751.43,1769.70,
    1796.16,1838.63,1939.65,2127.05,2225.54,2270.46,2307.71,2339.56,
    2366.73,2389.90,2409.76,
  tprint=1738.22,1939.65,2389.90, &end

```

TABLE D.1.—Continued.

```

&start p=1.730, mach=2.0, &end
CH4      0.049768
O2       0.199072
N2       0.75116
CN       0.0000001
END
&solver emax=1.0E-3, atolsp=1.0E-12, mf=21, &end
FINIS
LSSENS  METHANE  AIR  MECHANISM  ASSIGNED (CONST.) TEMP. FLOW PROBLEM  CASE 9
REPEAT
DISTANCE PRESSURE
&prob  cx0=1.730, combus=.true., exchr=.false.,
print=25.0,42.0,48.0, &end
&tmpdat cx0=1700.0, &end
&start  area=1000.0, mach=2.0, &end
CH4      0.049768
O2       0.199072
N2       0.75116
CN       0.0000001
END
&solver emax=1.0E-4, atolsp=1.0E-13, &end
FINIS
LSSENS  METHANOL - AIR  COMBUSTION
NEW
M      + CH3OH = CH3 + OH      3.2E+18  0.      80000.
O2     + CH3OH = CH2OH + HO2    4.0E+13  0.      50900.
OH     + CH3OH = CH2OH + H2O    4.0E+12  0.      2000.
O      + CH3OH = CH2OH + OH     1.6E+12  0.      2300.
H      + CH3OH = CH2OH + H2     3.2E+13  0.      7000.
H      + CH3OH = CH3 + H2O     5.0E+12  0.      5300.
CH3    + CH3OH = CH2OH + CH4    2.0E+11  0.      9800.
HO2    + CH3OH = CH2OH + H2O2   6.3E+12  0.      19400.
M      + CH2OH = CH2O + H       2.5E+13  0.      29000.
O2     + CH2OH = CH2O + HO2     1.0E+12  0.      6000.
M      + CH4 = CH3 + H         2.0E+17  0.      88000.
H      + CH4 = CH3 + H2        1.26E+14  0.      11900.
CH4    + O2 = CH3 + HO2        7.94E+13  0.      56000.
O      + CH4 = CH3 + OH        1.9E+14  0.      11720.
OH     + CH4 = CH3 + H2O       2.5E+13  0.      5010.
CH3    + O2 = CH3O + O         2.4E+13  0.      28680.
CH3    + OH = CH3O + H         6.3E+12  0.      0.
M      + CH3O = CH2O + H        5.0E+13  0.      21000.
CH3    + CH3 = C2H6            2.4E+14  -.4      0.
H      + C2H6 = C2H5 + H2      1.32E+14  0.      9700.
O      + C2H6 = C2H5 + OH      1.13E+14  0.      7850.
OH     + C2H6 = C2H5 + H2O     8.7E+13  0.      3520.
M      + C2H5 = C2H4 + H        1.0E+17  0.      31000.
C2H5   + O2 = C2H4 + HO2       2.0E+12  0.      5000.
H      + C2H5 = C2H4 + H2      4.8E+13  0.      0.
CH3    + CH2 = C2H4 + H        2.0E+13  0.      0.
H      + C2H4 = H2 + C2H3      1.5E+14  0.      10200.
M      + C2H4 = C2H2 + H2       2.6E+17  0.      79300.
C2H4   + OH = C2H3 + H2O       4.8E+12  0.      1230.
C2H4   + OH = CH3 + CH2O       2.0E+12  0.      960.
C2H4   + O = CH3 + HCO         3.3E+12  0.      1130.
C2H4   + O = CH2O + CH2        2.5E+13  0.      5000.
M      + C2H3 = C2H2 + H        3.0E+15  0.      32000.
C2H3   + O2 = CH2O + HCO       3.98E+12  0.      -250.
C2H3   + H = C2H2 + H2         6.0E+12  0.      0.
C2H3   + O = C2H2O + H         3.3E+13  0.      0.
C2H3   + OH = C2H2 + H2O       5.0E+12  0.      0.
C2H3   + CH2 = C2H2 + CH3      3.0E+13  0.      0.
C2H3   + C2H = 2.0C2H2        3.0E+13  0.      0.
M      + C2H2 = C2H + H         4.2E+16  0.      107000.
C2H2   + O = CH2 + CO          1.6E+14  0.      9890.
C2H2   + O = C2HO + H          4.0E+14  0.0     10660.
C2H2   + OH = C2H + H2O       6.3E+12  0.0     7000.
C2H2   + OH = C2H2O + H       3.2E+11  0.0     200.
C2H    + O2 = C2HO + O         5.00E+13  0.      1500.
C2H    + OH = C2HO + H        2.0E+13  0.      0.
C2HO   + O2 = 2.0CO + OH      1.46E+12  0.      2500.
C2HO   + O = 2.0CO + H        1.202E+12  0.      0.
C2HO   + OH = 2.0HCO         1.0E+13  0.      0.
C2HO   + H = CH2 + CO          5.0E+13  0.      0.
C2HO   + CH2 = C2H3 + CO       3.0E+13  0.      0.
C2HO   + CH2 = CH2O + C2H      1.0E+13  0.      2000.
2.0C2HO = C2H2 + 2.0CO       1.0E+13  0.      0.
C2H2O  + OH = CH2O + HCO       2.8E+13  0.      0.
C2H2O  + OH = C2HO + H2O      7.5E+12  0.      3000.
C2H2O  + H = CH3 + CO          1.13E+13  0.      3428.
C2H2O  + H = C2HO + H2        7.5E+13  0.      8000.
C2H2O  + O = C2HO + OH        5.0E+13  0.      8000.

```

TABLE D.1.—Continued.

C2H2O	+	O	=	CH2O	+	CO	2.0E+13	0.	0.
M	+	C2H2O	=	CH2	+	CO	2.0E+16	0.	60000.
C2H	+	O	=	CO	+	CH	5.0E+13	0.	0.
CH3O	+	O2	=	CH2O	+	HO2	1.0E+13	0.	7170.
CH3O	+	H	=	CH2O	+	H2	2.0E+13	0.	0.
M	+	CH2O	=	HCO	+	H	5.0E+16	0.	81000.
CH2O	+	OH	=	HCO	+	H2O	3.0E+13	0.	1200.
CH2O	+	H	=	HCO	+	H2	2.5E+13	0.	3990.
CH2O	+	O	=	HCO	+	OH	3.5E+13	0.	3510.
CH3	+	CH2O	=	CH4	+	HCO	1.0E+10	0.5	6000.
CH3	+	HCO	=	CH4	+	CO	3.0E+11	.5	0.
CH3	+	HO2	=	CH3O	+	OH	2.0E+13	0.	0.
M	+	CH3	=	CH2	+	H	1.95E+16	0.	91600.
H	+	CH3	=	H2	+	CH2	2.7E+11	.67	25700.
O	+	CH3	=	OH	+	CH2	1.9E+11	.68	25700.
OH	+	CH3	=	H2O	+	CH2	2.7E+11	.67	25700.
CH	+	CO2	=	HCO	+	CO	3.7E+12	0.	0.
CH	+	O2	=	HCO	+	O	1.0E+13	0.	0.
CH2	+	O2	=	CH2O	+	O	5.0E+11	0.5	6960.
CH2	+	O	=	CH	+	OH	2.0E+11	.7	25800.
CH2	+	OH	=	CH	+	H2O	5.0E+11	.5	5900.
CH2	+	H	=	CH	+	H2	3.2E+11	0.7	4970.
CH2	+	CH2	=	C2H3	+	H	5.0E+12	0.	0.
CH2	+	CH2	=	C2H2	+	H2	4.0E+13	0.	0.
HCO	+	O2	=	CO	+	HO2	3.0E+13	0.	0.
HCO	+	O	=	CO	+	OH	3.0E+13	0.	0.
HCO	+	OH	=	CO	+	H2O	3.0E+13	0.	0.
HCO	+	H	=	CO	+	H2	2.0E+13	0.	0.
M	+	HCO	=	H	+	CO	2.9E+14	0.	15570.
CO	+	O	=	CO2	+	M	2.4E+15	0.	4100.
CO	+	O2	=	CO2	+	O	2.5E+12	0.	47690.
CO	+	OH	=	CO2	+	H	4.17E+11	0.	1000.
CO	+	HO2	=	CO2	+	OH	5.75E+13	0.	22930.
O	+	H2O	=	OH	+	OH	6.8E+13	0.	18365.
H	+	O2	=	OH	+	O	1.89E+14	0.	16400.
O	+	H2	=	OH	+	H	4.20E+14	0.	13750.
H	+	HO2	=	H2	+	O2	7.28E+13	0.	2126.
O	+	HO2	=	OH	+	O2	5.0E+13	0.	1000.
HO2	+	OH	=	H2O	+	O2	8.0E+12	0.	0.
H	+	HO2	=	2.0OH			1.34E+14	0.	1070.
H2	+	HO2	=	H2O2	+	H	7.91E+13	0.	25000.
OH	+	H2O2	=	H2O	+	HO2	6.1E+12	0.	1430.
HO2	+	HO2	=	H2O2	+	O2	1.8E+12	0.	0.
H	+	H2O2	=	OH	+	H2O	7.8E+11	0.	0.
M	+	H2O2	=	2.0OH			1.44E+17	0.	45510.
THIRDBODY									
H2		2.30	O2		.78	H2O	6.0	H2O2	6.6
END									
H2	+	OH	=	H2O	+	H	4.74E+13	0.	6098.
H	+	O2	=	HO2	+	M	1.46E+15	0.	-1000.
THIRDBODY									
O2		1.30	N2		1.3	H2O	21.3	CO2	7.0
END									
M	+	H2O	=	H	+	OH	1.30E+15	0.	105140.
THIRDBODY									
H2		4.00	O2		1.5	H2O	20.0	N2	1.5
CO2		4.0	END						
H	+	O	=	OH	+	M	7.1E+18	-1.	0.
M	+	H2	=	H	+	H	2.2E+14	0.	96000.
THIRDBODY									
H2		4.10	O2		2.0	H2O	15.0	N2	2.0
END									
M	+	O2	=	O	+	O	1.80E+18	-1.	118020.
CH	+	N2	=	HCN	+	N	1.0E+11	0.	19000.
CN	+	H2	=	HCN	+	H	6.0E+13	0.	5300.
O	+	HCN	=	OH	+	CN	1.4E+11	.68	16900.
OH	+	HCN	=	HNCO	+	H	4.0E+11	0.	2800.
CN	+	O	=	CO	+	N	1.2E+13	0.	0.
CN	+	OH	=	NCO	+	H	2.5E+14	0.	6000.
H2	+	NCO	=	HNCO	+	H	1.0E+14	0.	9000.
HNCO	+	H	=	NH2	+	CO	1.0E+14	0.	8500.
CN	+	O2	=	NCO	+	O	3.2E+13	0.	1000.
CN	+	CO2	=	NCO	+	CO	3.7E+12	0.	0.
O	+	NCO	=	NO	+	CO	2.0E+13	0.	0.
N	+	NCO	=	N2	+	CO	1.0E+13	0.	0.
H	+	NCO	=	NH	+	CO	2.0E+13	0.	0.
CH	+	NO	=	N	+	HCO	1.6E+13	0.	9940.
CH	+	NO	=	O	+	HCN	2.0E+12	0.	0.
NH	+	OH	=	N	+	H2O	5.0E+11	0.5	2000.
HO2	+	NO	=	NO2	+	OH	2.09E+12	0.	-477.
O	+	NO2	=	NO	+	O2	1.0E+13	0.	596.
NO	+	O	=	NO2	+	M	5.62E+15	0.	-1160.

TABLE D.1.—Continued.

NO2	+	H	=	NO	+	OH	3.47E+14	0.	1470.
NO	+	H	=	N	+	OH	2.63E+14	0.	50410.
NO	+	O	=	N	+	O2	3.8E+9	1.	41370.
O	+	N2	=	NO	+	N	1.80E+14	0.	76250.
N	+	NO2	=	2.CNO			4.0E+12	0.	0.
M	+	N2O	=	N2	+	O	6.92E+23	-2.5	65000.
O	+	N2O	=	N2	+	O2	1.0E+14	0.	28020.
O	+	N2O	=	2.ONO			6.92E+13	0.	26630.
N2O	+	H	=	N2	+	OH	7.59E+13	0.	15100.
NO2	+	H2	=	HNO2	+	H	2.4E+13	0.	29000.
OH	+	NO2	=	HNO3	+	M	3.0E+15	0.	-3800.
THIRDBODY									
O2		0.70		H2		1.4		END	
OH	+	NO	=	HNO2	+	M	5.6E+15	0.	-1700.
HNO	+	H	=	H2	+	NO	5.0E+12	0.	0.
H	+	NO	=	HNO	+	M	5.4E+15	0.	-600.
HNO	+	OH	=	H2O	+	NO	3.6E+13	0.	0.
AR									
TIME									
CH3OH									
&prob rhocon=.true., print=4.0E-4,5.0E-4,6.5E-4, &end									
&start t=1300.0, mmhg=.true., p=760.0, eratio=2.0, scc=1.0,									
sch=4.0, scox=1.0, &end									
CN		0.000001							
CH		0.00001							
N		0.000001							
END									
&solver emax=5.0E-4, atolsp=1.0E-12, &end									
FINIS									
LSENS PROPANE-AIR WELL-STIRRED REACTOR + ROCKET EXP; EMAX=10-4 CASE 11									
NEW									
CH3	+	C3H8	=	C2H5	+	CH3	5.0E+15	0.	83500.
		C3H8	=	CH4	+	C3H7	3.55E+12	0.	10300.
		C3H7	=	C2H4	+	CH3	3.0E+14	0.	33200.
M	+	CH4	=	CH3	+	H	2.0E+17	0.	88000.
H	+	CH4	=	CH3	+	H2	1.26E+14	0.	11900.
CH4	+	O2	=	CH3	+	HO2	7.94E+13	0.	56000.
O	+	CH4	=	CH3	+	OH	1.9E+14	0.	11720.
OH	+	CH4	=	CH3	+	H2O	2.5E+13	0.	5010.
CH3	+	O2	=	CH3O	+	O	2.4E+13	0.	28680.
CH3	+	OH	=	CH3O	+	H	6.3E+12	0.	0.
M	+	CH3O	=	CH2O	+	H	5.0E+13	0.	21000.
CH3	+	CH3	=	C2H6			2.4E+14	-4	0.
H	+	C2H6	=	C2H5	+	H2	1.32E+14	0.	9700.
O	+	C2H6	=	C2H5	+	OH	1.13E+14	0.	7850.
OH	+	C2H6	=	C2H5	+	H2O	8.7E+13	0.	3520.
M	+	C2H5	=	C2H4	+	H	1.0E+17	0.	31000.
C2H5	+	O2	=	C2H4	+	HO2	2.0E+12	0.	5000.
H	+	C2H5	=	C2H4	+	H2	4.8E+13	0.	0.
CH3	+	CH2	=	C2H4	+	H	2.0E+13	0.	0.
H	+	C2H4	=	H2	+	C2H3	1.5E+14	0.	10200.
M	+	C2H4	=	C2H2	+	H2	2.6E+17	0.	79300.
C2H4	+	OH	=	C2H3	+	H2O	4.8E+12	0.	1230.
C2H4	+	OH	=	CH3	+	CH2O	2.0E+12	0.	960.
C2H4	+	O	=	CH3	+	HCO	3.3E+12	0.	1130.
C2H4	+	O	=	CH2O	+	CH2	2.5E+13	0.	5000.
M	+	C2H3	=	C2H2	+	H	3.0E+15	0.	32000.
C2H3	+	O2	=	CH2O	+	HCO	3.98E+12	0.	-250.
C2H3	+	H	=	C2H2	+	H2	6.0E+12	0.	0.
C2H3	+	O	=	C2H2O	+	H	3.3E+13	0.	0.
C2H3	+	OH	=	C2H2	+	H2O	5.0E+12	0.	0.
C2H3	+	CH2	=	C2H2	+	CH3	3.0E+13	0.	0.
C2H3	+	C2H	=	2.0C2H2			3.0E+13	0.	0.
M	+	C2H2	=	C2H	+	H	4.2E+16	0.	107000.
C2H2	+	O	=	CH2	+	CO	1.6E+14	0.	9890.
C2H2	+	O	=	C2HO	+	H	4.0E+14	0.0	10660.
C2H2	+	OH	=	C2H	+	H2O	6.3E+12	0.0	7000.
C2H2	+	OH	=	C2H2O	+	H	3.2E+11	0.0	200.
C2H	+	O2	=	C2HO	+	O	5.00E+13	0.	1500.
C2H	+	OH	=	C2HO	+	H	2.0E+13	0.	0.
C2HO	+	O2	=	2.0CO	+	OH	1.46E+12	0.	2500.
C2HO	+	O	=	2.0CO	+	H	1.202E+12	0.	0.
C2HO	+	OH	=	2.0HCO			1.0E+13	0.	0.
C2HO	+	H	=	CH2	+	CO	5.0E+13	0.	0.
C2HO	+	CH2	=	C2H3	+	CO	3.0E+13	0.	0.
C2HO	+	CH2	=	CH2O	+	C2H	1.0E+13	0.	2000.
		2.0C2HO	=	C2H2	+	2.0CO	1.0E+13	0.	0.
C2H2O	+	OH	=	CH2O	+	HCO	2.8E+13	0.	0.
C2H2O	+	OH	=	C2HO	+	H2O	7.5E+12	0.	3000.
C2H2O	+	H	=	CH3	+	CO	1.13E+13	0.	3428.
C2H2O	+	H	=	C2HO	+	H2	7.5E+13	0.	8000.
C2H2O	+	O	=	C2HO	+	OH	5.0E+13	0.	8000.

TABLE D.1.—Continued.

C2H2O	+	O	=	CH2O	+	CO	2.0E+13	0.	0.
M	+	C2H2O	=	CH2	+	CO	2.0E+16	0.	60000.
C2H	+	O	=	CO	+	CH	5.0E+13	0.	0.
CH3O	+	O2	=	CH2O	+	HO2	1.0E+13	0.	7170.
CH3O	+	H	=	CH2O	+	H2	2.0E+13	0.	0.
M	+	CH2O	=	HCO	+	H	5.0E+16	0.	81000.
CH2O	+	OH	=	HCO	+	H2O	3.0E+13	0.	1200.
CH2O	+	H	=	HCO	+	H2	2.5E+13	0.	3990.
CH2O	+	O	=	HCO	+	OH	3.5E+13	0.	3510.
CH3	+	CH2O	=	CH4	+	HCO	1.0E+10	0.5	6000.
CH3	+	HCO	=	CH4	+	CO	3.0E+11	.5	0.
CH3	+	HO2	=	CH3O	+	OH	2.0E+13	0.	0.
M	+	CH3	=	CH2	+	H	1.95E+16	0.	91600.
H	+	CH3	=	H2	+	CH2	2.7E+11	.67	25700.
O	+	CH3	=	OH	+	CH2	1.9E+11	.68	25700.
OH	+	CH3	=	H2O	+	CH2	2.7E+11	.67	25700.
CH	+	CO2	=	HCO	+	CO	3.7E+12	0.	0.
CH	+	O2	=	HCO	+	O	1.0E+13	0.	0.
CH2	+	O2	=	CH2O	+	O	5.0E+11	0.5	6960.
CH2	+	O	=	CH	+	OH	2.0E+11	.7	25800.
CH2	+	OH	=	CH	+	H2O	5.0E+11	.5	5900.
CH2	+	H	=	CH	+	H2	3.2E+11	0.7	4970.
CH2	+	CH2	=	C2H3	+	H	5.0E+12	0.	0.
CH2	+	CH2	=	C2H2	+	H2	4.0E+13	0.	0.
HCO	+	O2	=	CO	+	HO2	3.0E+13	0.	0.
HCO	+	O	=	CO	+	OH	3.0E+13	0.	0.
HCO	+	OH	=	CO	+	H2O	3.0E+13	0.	0.
HCO	+	H	=	CO	+	H2	2.0E+13	0.	0.
M	+	HCO	=	H	+	CO	2.9E+14	0.	15570.
CO	+	O	=	CO2	+	M	2.4E+15	0.	4100.
CO	+	O2	=	CO2	+	O	2.5E+12	0.	47690.
CO	+	OH	=	CO2	+	H	4.17E+11	0.	1000.
CO	+	HO2	=	CO2	+	OH	5.75E+13	0.	22930.
O	+	H2O	=	OH	+	OH	6.8E+13	0.	18365.
H	+	O2	=	OH	+	O	1.89E+14	0.	16400.
O	+	H2	=	OH	+	H	4.20E+14	0.	13750.
H	+	HO2	=	H2	+	O2	7.28E+13	0.	2126.
O	+	HO2	=	OH	+	O2	5.0E+13	0.	1000.
HO2	+	OH	=	H2O	+	O2	8.0E+12	0.	0.
H	+	HO2	=	2.0OH			1.34E+14	0.	1070.
H2	+	HO2	=	H2O2	+	H	7.91E+13	0.	25000.
OH	+	H2O2	=	H2O	+	HO2	6.1E+12	0.	1430.
HO2	+	HO2	=	H2O2	+	O2	1.8E+12	0.	0.
H	+	H2O2	=	OH	+	H2O	7.8E+11	0.	0.
M	+	H2O2	=	2.0OH			1.44E+17	0.	45510.
THIRDBODY									
H2		2.30	O2		.78	H2O	6.0	H2O2	6.6
END									
H2	+	OH	=	H2O	+	H	4.74E+13	0.	6098.
H	+	O2	=	HO2	+	M	1.46E+15	0.	-1000.
THIRDBODY									
O2		1.30	N2		1.3	H2O	21.3	CO2	7.0
END									
M	+	H2O	=	H	+	OH	1.30E+15	0.	105140.
THIRDBODY									
H2		4.00	O2		1.5	H2O	20.0	N2	1.5
CO2		4.0	END						
H	+	O	=	OH	+	M	7.1E+18	-1.	0.
M	+	H2	=	H	+	H	2.2E+14	0.	96000.
THIRDBODY									
H2		4.10	O2		2.0	H2O	15.0	N2	2.0
END									
M	+	O2	=	O	+	O	1.80E+18	-1.	118020.
CH	+	N2	=	HCN	+	N	1.0E+11	0.	19000.
CN	+	H2	=	HCN	+	H	6.0E+13	0.	5300.
O	+	HCN	=	OH	+	CN	1.4E+11	.68	16900.
OH	+	HCN	=	HNCO	+	H	4.0E+11	0.	2800.
CN	+	O	=	CO	+	N	1.2E+13	0.	0.
CN	+	OH	=	NCO	+	H	2.5E+14	0.	6000.
H2	+	NCO	=	HNCO	+	H	1.0E+14	0.	9000.
HNCO	+	H	=	NH2	+	CO	1.0E+14	0.	8500.
CN	+	O2	=	NCO	+	O	3.2E+13	0.	1000.
CN	+	CO2	=	NCO	+	CO	3.7E+12	0.	0.
O	+	NCO	=	NO	+	CO	2.0E+13	0.	0.
N	+	NCO	=	N2	+	CO	1.0E+13	0.	0.
H	+	NCO	=	NH	+	CO	2.0E+13	0.	0.
CH	+	NO	=	N	+	HCO	1.6E+13	0.	9940.
CH	+	NO	=	O	+	HCN	2.0E+12	0.	0.
NH	+	OH	=	N	+	H2O	5.0E+11	0.5	2000.
HO2	+	NO	=	NO2	+	OH	2.09E+12	0.	-477.
O	+	NO2	=	NO	+	O2	1.0E+13	0.	596.
NO	+	O	=	NO2	+	M	5.62E+15	0.	-1160.

TABLE D.1.—Continued.

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NO2      +      H      =      NO      +      OH      3.47E+14      0.      1470.
NO       +      H      =      N       +      OH      2.63E+14      0.      50410.
NO       +      O       =      N       +      O2      3.8E+9       1.      41370.
O        +      N2      =      NO      +      N       1.80E+14      0.      76250.
N        +      NO2     =2.0NO      +      N       4.0E+12      0.      0.
M        +      N2O     =      N2      +      O       6.92E+23      -2.5     65000.
O        +      N2O     =      N2      +      O2      1.0E+14      0.      28020.
O        +      N2O     =2.0NO      +      O       6.92E+13      0.      26630.
N2O      +      H       =      N2      +      OH      7.59E+13      0.      15100.
NO2      +      H2      =      HNO2     +      H       2.4E+13      0.      29000.
OH       +      NO2     =      HNO3     +      M       3.0E+15      0.      -3800.
THIRDBODY
O2       0.70      H2      1.4      END
OH       +      NO      =      HNO2     +      M       5.6E+15      0.      -1700.
HNO      +      H       =      H2      +      NO      5.0E+12      0.      0.
H        +      NO      =      HNO      +      M       5.4E+15      0.      -600.
HNO      +      OH      =      H2O      +      NO      3.6E+13      0.      0.

AR
DISTANCE AREA
&prob welstr=.true., conc=.false., wsflow=.true.,
  cx0=15.0, cxi=20.0, print=0.4,2.0,4.0, rocket=.true., htran=.true.,
  ht1=0.05, ht0=-42.88, pc= 73.5, athrot=2.325, &end
&wsprob dotmax=1600.0, delmd=800.0, mpr=1, volume=300.0,
  wsrhtr=.true., wsrht1=0.05, wsrht0=-42.88, &end
&start t=614.0, p=5.0, mdot=10.0, molef=.false., x=0.2, &end
C3H8     0.0873262
N2       0.6892887
O2       0.211232
AR       0.011737
CO2      0.0004162
END
&solver emax=1.0E-4, atolsp=1.0E-13, &end
FINIS
LSSENS   HIGH TEMPERATURE AIR IONIZATION                                CASE 12
NEW
N        +      O2      =      NO      +      O       6.4E+09      1.      6250.
O        +      N2      =      NO      +      N       1.8E+14      0.      76250.
N        +      O       =      NO      +      M       6.40E+16      -0.5     0.
THIRDBODY
N2O      2.25      END
O        +      O       =      O2      +      M       5.7E+13      0.      -1790.
M        +      N2      =      N       +      N       3.72E+21      -1.6     225000.
NO       +      O       =      NO2     +      M       5.62E+15      0.      -1160.
THIRDBODY
N2       1.55      END
M        +      N2O     =      N2      +      O       6.92E+23      -2.5     65000.
O        +      N2O     =      N2      +      O2      1.0E+14      0.      28020.
NO+      +      E       =      N       +      O       1.45E+21      -1.5     0.
O+       +      E       =      O       +      M       2.00E+26      -2.5     0.
THIRDBODY
O2       4.50      N       0.03      NO      50.0      O       .03
END
O2       +      E       =      O2-     +      M       1.52E+21      -1.      1190.
THIRDBODY
N2       .000002      END
O2       +      O-      =      O2-     +      O       6.00E+12      0.      0.

END
DISTANCE AREA
&prob cx0=1000.0, dbugo=.true., order=.true.,
  print=0.06,0.50,0.70, &end
&start p=1.6803, v=47002.0, t=4820.0, &end
N2       0.7905
O2       0.2095
O2-      0.0000000001
END
&solver emax=1.0E-3, atolsp=1.0E-12, &end
FINIS
LSSENS   HIGH PRESSURE HYDROGEN - CARBON MONOXIDE REACTION            CASE 13
NEW
CH3      +      OH      =      CH3O     +      H       6.3E+12      0.      0.
M        +      CH3O     =      CH2O     +      H       5.0E+13      0.      21000.
CH3O     +      H       =      CH2O     +      H2      2.0E+13      0.      0.
CH3      +      HCO      =      CH4      +      CO      3.0E+11      .5      0.
CH3      +      HO2      =      CH3O     +      OH      2.0E+13      0.      0.
M        +      CH4      =      CH3      +      H       2.0E+17      0.      88000.
H        +      CH4      =      CH3      +      H2      1.26E+14      0.      11900.
OH       +      CH4      =      CH3      +      H2O     2.5E+13      0.      5010.
CH2O     +      H       =      HCO      +      H2      2.5E+13      0.      3990.
CH2O     +      OH      =      HCO      +      H2O     3.0E+13      0.      1200.
M        +      CH2O     =      H       +      HCO     5.0E+16      0.      81000.

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TABLE D.1.—Continued.

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HCO      +      H      =      CO      +      H2      2.0E+13      0.      0.
HCO      +      OH      =      CO      +      H2O      3.0E+13      0.      0.
M        +      HCO      =      H      +      CO      2.9E+14      0.      15570.
CO       +      OH      =      CO2     +      H      4.17E+11      0.0     1000.
CO       +      HO2     =      CO2     +      OH      5.75E+13      0.      22930.
H        +      HO2     =2.0OH      1.34E+14      0.      1070.
H2       +      HO2     =      H2O2    +      H      7.91E+13      0.      25000.
OH       +      H2O2    =      H2O     +      HO2     6.1E+12      0.      1430.
M        +      H2O2    =2.0OH      1.44E+17      0.      45510.
THIRDBODY
H2       2.30      H2O2     6.6      H2O      6.0      END
H2       +      OH      =      H2O     +      H      4.74E+13      0.      6098.
M        +      H2O     =      H      +      OH      1.30E+15      0.      105140.
THIRDBODY
H2       4.00      CO2      4.0      H2O      20.0      END
M        +      H2      =      H      +      H      2.2E+14      0.      96000.
THIRDBODY
H2       4.10      H2O      15.0      END

END
TIME
&prob print=1.0,1.E+6,1.E+8,1.E+9, combus=.true.,
rhocon=.true., tcon=.true., &end
&start t=1000.0, p=100.0, &end
H2      0.99
CO      0.01
END
&solver emax=1.0E-3, atolsp=1.0E-12, &end
FINIS
LSENS   HYDROGEN - OXYGEN LOW TEMPERATURE PHOTOLYTIC IGNITION      CASE 14
NEW
O        +      H2O      =      OH      +      OH      6.8E+13      0.      18365.
H        +      O2       =      OH      +      O      1.89E+14      0.      16400.
O        +      H2       =      OH      +      H      4.20E+14      0.      13750.
H        +      HO2     =      H2      +      O2     7.28E+13      0.      2126.
O        +      HO2     =      OH      +      O2     5.0E+13      0.      1000.
HO2      +      OH      =      H2O     +      O2     8.0E+12      0.      0.
H        +      HO2     =2.0OH      1.34E+14      0.      1070.
H2       +      HO2     =      H2O2    +      H      7.91E+13      0.      25000.
OH       +      H2O2    =      H2O     +      HO2     6.1E+12      0.      1430.
HO2      +      HO2     =      H2O2    +      O2     1.8E+12      0.      0.
H        +      H2O2    =      OH      +      H2O     7.8E+11      0.      0.
M        +      H2O2    =      OH      +      OH      1.44E+17      0.      45510.
THIRDBODY
H2       2.30      O2       .78      H2O      6.0      H2O2     6.6
END
H2       +      OH      =      H2O     +      H      4.74E+13      0.      6098.
H        +      O2       =      HO2     +      M      1.46E+15      0.      -1000.
THIRDBODY
O2       1.30      H2      3.0      H2O      21.3      END
M        +      H2O     =      H      +      OH      1.30E+15      0.      105140.
THIRDBODY
H2       4.00      O2      1.5      H2O      20.0      END
H        +      O        =      OH      +      M      7.1E+18      -1.      0.
M        +      H2      =      H      +      H      2.2E+14      0.      96000.
THIRDBODY
H2       4.10      O2      2.0      H2O      15.0      END
M        +      O2      =      O        +      O      1.80E+18      -1.      118020.
HNU      +      H2      >2.0H      .003      0.      0.
HNU      +      O2      >2.0O      .005      0.      0.

END
TIME
&prob rhocon=.true., iprint=100, combus=.true., end=1.0173, &end
&start t=700.0, p=2.0, &end
H2      0.667
O2      0.333
END
&solver emax=1.0E-6, atolsp=1.0E-11, &end
FINIS
LSENS   METHANE IR MECHAN.; MON. DECR. TABULAR AREA WITH APRINT      CASE 15
NEW
M        +      CH4      =      CH3      +      H      2.0E+17      0.      88000.
H        +      CH4      =      CH3      +      H2     1.26E+14      0.      11900.
CH4      +      O2       =      CH3      +      HO2     7.94E+13      0.      56000.
O        +      CH4      =      CH3      +      OH      1.9E+14      0.      11720.
OH       +      CH4      =      CH3      +      H2O     2.5E+13      0.      5010.
CH3      +      O2       =      CH3O     +      O      2.4E+13      0.      28680.
CH3      +      OH      =      CH3O     +      H      6.3E+12      0.      0.
M        +      CH3O     =      CH2O     +      H      5.0E+13      0.      21000.
CH3      +      CH3      =      C2H6     +      H2     2.4E+14      -1.4     0.
H        +      C2H6     =      C2H5     +      H2     1.32E+14      0.      9700.

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TABLE D.1.—Continued.

O	+	C2H6	=	C2H5	+	OH	1.13E+14	0.	7850.
OH	+	C2H6	=	C2H5	+	H2O	8.7E+13	0.	3520.
M	+	C2H5	=	C2H4	+	H	1.0E+17	0.	31000.
C2H5	+	O2	=	C2H4	+	HO2	2.0E+12	0.	5000.
H	+	C2H5	=	C2H4	+	H2	4.8E+13	0.	0.
CH3	+	CH2	=	C2H4	+	H	2.0E+13	0.	0.
H	+	C2H4	=	H2	+	C2H3	1.5E+14	0.	10200.
M	+	C2H4	=	C2H2	+	H2	2.6E+17	0.	79300.
C2H4	+	OH	=	C2H3	+	H2O	4.8E+12	0.	1230.
C2H4	+	OH	=	CH3	+	CH2O	2.0E+12	0.	960.
C2H4	+	O	=	CH3	+	HCO	3.3E+12	0.	1130.
C2H4	+	O	=	CH2O	+	CH2	2.5E+13	0.	5000.
M	+	C2H3	=	C2H2	+	H	3.0E+15	0.	32000.
C2H3	+	O2	=	CH2O	+	HCO	3.98E+12	0.	-250.
C2H3	+	H	=	C2H2	+	H2	6.0E+12	0.	0.
C2H3	+	O	=	C2H2O	+	H	3.3E+13	0.	0.
C2H3	+	OH	=	C2H2	+	H2O	5.0E+12	0.	0.
C2H3	+	CH2	=	C2H2	+	CH3	3.0E+13	0.	0.
C2H3	+	C2H	=	2.0C2H2			3.0E+13	0.	0.
M	+	C2H2	=	C2H	+	H	4.2E+16	0.	107000.
C2H2	+	O	=	CH2	+	CO	1.6E+14	0.	9890.
C2H2	+	O	=	C2HO	+	H	4.0E+14	0.0	10660.
C2H2	+	OH	=	C2H	+	H2O	6.3E+12	0.0	7000.
C2H2	+	OH	=	C2H2O	+	H	3.2E+11	0.0	200.
C2H	+	O2	=	C2HO	+	O	5.00E+13	0.	1500.
C2H	+	OH	=	C2HO	+	H	2.0E+13	0.	0.
C2HO	+	O2	=	2.0CO	+	OH	1.46E+12	0.	2500.
C2HO	+	O	=	2.0CO	+	H	1.202E+12	0.	0.
C2HO	+	OH	=	2.0HCO			1.0E+13	0.	0.
C2HO	+	H	=	CH2	+	CO	5.0E+13	0.	0.
C2HO	+	CH2	=	C2H3	+	CO	3.0E+13	0.	0.
C2HO	+	CH2	=	CH2O	+	C2H	1.0E+13	0.	2000.
C2HO	+	2.0C2HO	=	C2H2	+	2.0CO	1.0E+13	0.	0.
C2H2O	+	OH	=	CH2O	+	HCO	2.8E+13	0.	0.
C2H2O	+	OH	=	C2HO	+	H2O	7.5E+12	0.	3000.
C2H2O	+	H	=	CH3	+	CO	1.13E+13	0.	3428.
C2H2O	+	H	=	C2HO	+	H2	7.5E+13	0.	8000.
C2H2O	+	O	=	C2HO	+	OH	5.0E+13	0.	8000.
C2H2O	+	O	=	CH2O	+	CO	2.0E+13	0.	0.
M	+	C2H2O	=	CH2	+	CO	2.0E+16	0.	60000.
C2H	+	O	=	CO	+	CH	5.0E+13	0.	0.
CH3O	+	O2	=	CH2O	+	HO2	1.0E+13	0.	7170.
CH3O	+	H	=	CH2O	+	H2	2.0E+13	0.	0.
M	+	CH2O	=	HCO	+	H	5.0E+16	0.	81000.
CH2O	+	OH	=	HCO	+	H2O	3.0E+13	0.	1200.
CH2O	+	H	=	HCO	+	H2	2.5E+13	0.	3990.
CH2O	+	O	=	HCO	+	OH	3.5E+13	0.	3510.
CH3	+	CH2O	=	CH4	+	HCO	1.0E+10	0.5	6000.
CH3	+	HCO	=	CH4	+	CO	3.0E+11	.5	0.
CH3	+	HO2	=	CH3O	+	OH	2.0E+13	0.	0.
M	+	CH3	=	CH2	+	H	1.95E+16	0.	91600.
H	+	CH3	=	H2	+	CH2	2.7E+11	.67	25700.
O	+	CH3	=	OH	+	CH2	1.9E+11	.68	25700.
OH	+	CH3	=	H2O	+	CH2	2.7E+11	.67	25700.
CH	+	CO2	=	HCO	+	CO	3.7E+12	0.	0.
CH	+	O2	=	HCO	+	O	1.0E+13	0.	0.
CH2	+	O2	=	CH2O	+	O	5.0E+11	0.5	6960.
CH2	+	O	=	CH	+	OH	2.0E+11	.7	25800.
CH2	+	OH	=	CH	+	H2O	5.0E+11	.5	5900.
CH2	+	H	=	CH	+	H2	3.2E+11	0.7	4970.
CH2	+	CH2	=	C2H3	+	H	5.0E+12	0.	0.
CH2	+	CH2	=	C2H2	+	H2	4.0E+13	0.	0.
HCO	+	O2	=	CO	+	HO2	3.0E+13	0.	0.
HCO	+	O	=	CO	+	OH	3.0E+13	0.	0.
HCO	+	OH	=	CO	+	H2O	3.0E+13	0.	0.
HCO	+	H	=	CO	+	H2	2.0E+13	0.	0.
M	+	HCO	=	H	+	CO	2.9E+14	0.	15570.
CO	+	O	=	CO2	+	M	2.4E+15	0.	4100.
CO	+	O2	=	CO2	+	O	2.5E+12	0.	47690.
CO	+	OH	=	CO2	+	H	4.17E+11	0.	1000.
CO	+	HO2	=	CO2	+	OH	5.75E+13	0.	22930.
O	+	H2O	=	OH	+	OH	6.8E+13	0.	18365.
H	+	O2	=	OH	+	O	1.89E+14	0.	16400.
O	+	H2	=	OH	+	H	4.20E+14	0.	13750.
H	+	HO2	=	H2	+	O2	7.28E+13	0.	2126.
O	+	HO2	=	OH	+	O2	5.0E+13	0.	1000.
HO2	+	OH	=	H2O	+	O2	8.0E+12	0.	0.
H	+	HO2	=	2.0OH			1.34E+14	0.	1070.
H2	+	HO2	=	H2O2	+	H	7.91E+13	0.	25000.
OH	+	H2O2	=	H2O	+	HO2	6.1E+12	0.	1430.
HO2	+	HO2	=	H2O2	+	O2	1.8E+12	0.	0.
H	+	H2O2	=	OH	+	H2O	7.8E+11	0.	0.

TABLE D.1.—Continued.

M	+	H2O2	=	2.OOH		1.44E+17	0.	45510.	
THIRDBODY									
H2		2.30	O2		.78	H2O	6.0	H2O2	6.6
END									
H2	+	OH	=	H2O	+	H	4.74E+13	0.	6098.
H	+	O2	=	HO2	+	M	1.46E+15	0.	-1000.
THIRDBODY									
O2		1.30	N2		1.3	H2O	21.3	CO2	7.0
END									
M	+	H2O	=	H	+	OH	1.30E+15	0.	105140.
THIRDBODY									
H2		4.00	O2		1.5	H2O	20.0	N2	1.5
CO2		4.0	END						
H	+	O	=	OH	+	M	7.1E+18	-1.	0.
M	+	H2	=	H	+	H	2.2E+14	0.	96000.
THIRDBODY									
H2		4.10	O2		2.0	H2O	15.0	N2	2.0
END									
M	+	O2	=	O	+	O	1.80E+18	-1.	118020.
CH	+	N2	=	HCN	+	N	1.0E+11	0.	19000.
CN	+	H2	=	HCN	+	H	6.0E+13	0.	5300.
O	+	HCN	=	OH	+	CN	1.4E+11	.68	16900.
OH	+	HCN	=	HNCO	+	H	4.0E+11	0.	2800.
CN	+	O	=	CO	+	N	1.2E+13	0.	0.
CN	+	OH	=	NCO	+	H	2.5E+14	0.	6000.
H2	+	NCO	=	HNCO	+	H	1.0E+14	0.	9000.
HNCO	+	H	=	NH2	+	CO	1.0E+14	0.	8500.
CN	+	O2	=	NCO	+	O	3.2E+13	0.	1000.
CN	+	CO2	=	NCO	+	CO	3.7E+12	0.	0.
O	+	NO	=	NO	+	CO	2.0E+13	0.	0.
N	+	NCO	=	N2	+	CO	1.0E+13	0.	0.
H	+	NCO	=	NH	+	CO	2.0E+13	0.	0.
CH	+	NO	=	N	+	HCO	1.6E+13	0.	9940.
CH	+	NO	=	O	+	HCN	2.0E+12	0.	0.
NH	+	OH	=	N	+	H2O	5.0E+11	0.5	2000.
HO2	+	NO	=	NO2	+	OH	2.09E+12	0.	-477.
O	+	NO2	=	NO	+	O2	1.0E+13	0.	596.
NO	+	O	=	NO2	+	M	5.62E+15	0.	-1160.
NO2	+	H	=	NO	+	OH	3.47E+14	0.	1470.
NO	+	H	=	N	+	OH	2.63E+14	0.	50410.
NO	+	O	=	N	+	O2	3.8E+9	1.	41370.
O	+	N2	=	NO	+	N	1.80E+14	0.	76250.
N	+	NO2	=	2.OONO			4.0E+12	0.	0.
M	+	N2O	=	N2	+	O	6.92E+23	-2.5	65000.
O	+	N2O	=	N2	+	O2	1.0E+14	0.	28020.
O	+	N2O	=	2.OONO			6.92E+13	0.	26630.
N2O	+	H	=	N2	+	OH	7.59E+13	0.	15100.
NO2	+	H2	=	HNO2	+	H	2.4E+13	0.	29000.
OH	+	NO2	=	HNO3	+	M	3.0E+15	0.	-3800.
THIRDBODY									
O2		0.70	H2		1.4	END			
OH	+	NO	=	HNO2	+	M	5.6E+15	0.	-1700.
HNO	+	H	=	H2	+	NO	5.0E+12	0.	0.
H	+	NO	=	HNO	+	M	5.4E+15	0.	-600.
HNO	+	OH	=	H2O	+	NO	3.6E+13	0.	0.

END

DISTANCE AREA

```
&prob xtb= 0.0,5.0,10.0,15.0,20.0,25.0,30.0,32.0,34.0,36.0,38.0,40.0,42.0,44.0,
atb= 1200.0,1180.0,1160.0,1140.0,1120.0,1100.0,1080.0,1060.0,1040.0,1020.0,
1000.0, 980.0, 960.0, 940.0,
```

```
aprint = 1180.0, 1150., 1110., 950.0, &end
```

```
&start t=1600.0, mach=2.0, p=1.730, &end
```

```
CH4 0.049768
```

```
O2 0.199072
```

```
N2 0.75116
```

```
CN 0.0000001
```

END

```
&solver emax=1.0E-5, atolsp=1.0E-14, &end
```

FINIS

```
LSENS METHANE - AIR WITH TAB. AREA PROFILE OF CASE 15, BUT PRINT ASSIG; CASE 16
```

REPEAT

DISTANCE AREA

```
&prob xtb= 0.0,5.0,10.0,15.0,20.0,25.0,30.0,32.0,34.0,36.0,38.0,40.0,42.0,44.0,
atb= 1200.0,1180.0,1160.0,1140.0,1120.0,1100.0,1080.0,1060.0,1040.0,1020.0,
1000.0, 980.0, 960.0, 940.0,
```

```
print = 5.0, 12.4954, 22.4363, 43.0002, &end
```

```
&start t=1600.0, mach=2.0, p=1.730, &end
```

```
CH4 0.049768
```

```
O2 0.199072
```

```
N2 0.75116
```

```
CN 0.0000001
```

TABLE D.1.--Concluded.

```
END
&solver  emax=1.0E-5, atolsp=1.0E-14,  &end
FINIS
```

(a) Case 1

COMPUTATIONAL WORK REQUIRED FOR EQUILIBRIUM SHOCK CALCULATION:
NO. OF ITERATIONS = 2 CPU TIME = 1.999998E-02 S

TABLE D.2.—Continued
(a) Continued.

** FROZEN SHOCK CALCULATION **			
	INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE (ATM)	0.1227	1.6017	13.0535
VELOCITY (CM/SEC)	57877.96	18411.41	0.3181
DENSITY (G/CM**3)	6.56043E-04	2.06203E-03	3.1436
TEMPERATURE (DEG K)	299.90	1249.31	4.1524
ENTHALPY (CAL/G)	0.62802	36.60887	58.29243
INTERNAL ENERGY (CAL/G)	-3.90133	17.80106	-4.56282
SP. HEAT (CP) (CAL/G/DEG K)	0.03804	0.03807	1.00084
ENTROPY (CAL/G/DEG K)	0.3422	0.3575	1.0449
MACH NUMBER	3.2646	0.5098	0.1562
GAMMA	1.6586	1.6577	0.9994
SONIC VELOCITY (CM/SEC)	17728.96	36117.20	2.0372
		SPECIES	MOLE FRACTION
		BR2	1.00000E-02
		BR	0.00000E+00
		XE	9.90000E-01
MIXTURE MOLECULAR WEIGHT		131.57527	
D(LOG VOLUME)/D(LOG T) AT CONSTANT P		1.0000	
D(LOG VOLUME)/D(LOG P) AT CONSTANT T		-1.0000	
COMPUTATIONAL WORK REQUIRED FOR FROZEN SHOCK CALCULATION. NO. OF ITERATIONS = 2 CPU TIME = 0.000000E+00 S			
DISTANCE-AREA VERSION	LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM		NASA LEWIS RESEARCH CENTER
	LSENS BROMINE DISSOCIATION IN A SHOCK TUBE		CASE 1
REACTION NUMBER	REACTION	REACTION RATE VARIABLES A N	ACTIVATION ENERGY
1	M + 1*BR2 = 2*BR	6.99000E+11 0.5000	35500.00
ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING			
M(BR2 , 1) = 3.80000			
** NEW INPUT DATA GIVEN IN CGS UNITS **			
** OUTPUT REQUIRED IN CGS UNITS **			
** ASSIGNED VARIABLE PROFILE **			
THE AREA IS CALCULATED FROM THE FOLLOWING FUNCTION (SHOCK TUBE CROSS-SECTIONAL AREA)/(AREA) = 1 - (X (CM)/ 32200.000)**(0.50000)			
NUMBER OF REACTING SPECIES: 2			
NUMBER OF INERT SPECIES: 1			
NUMBER OF SPECIES ODE'S REQUIRED FOR THIS CASE: 2			
TOTAL NUMBER OF ODE'S REQUIRED FOR THIS CASE: 5			
INTEGRATION CONTROLS			
INTEGRATION METHOD (MF): 21	MAXIMUM RELATIVE ERROR: 1.00000E-12	SPECIES ABSOLUTE ERROR:	1.00000E-10
MAXIMUM NUMBER OF STEPS ALLOWED FOR THE COMPLETE PROBLEM: 2000			
** OUTPUT REQUIRED AT FOLLOWING 3 PRINT STATIONS **			
	STATION	AXIAL DISTANCE (CM)	
	1	5.00000E-02	
	2	2.00000E+00	
	3	4.00000E+00	

TABLE D.2.—Continued.
(a) Continued.

** INITIAL CONDITIONS **							
TIME	0.00000E+00	SEC	AREA	1.00000E+00	AXIAL POSITION	0.00000E+00	CM
FLOW PROPERTIES				INTEGRATION INDICATORS			
PRESSURE (ATM)	1.60167			STEPS FROM LAST PRINT		0	
VELOCITY (CM/SEC)	18411.41			AVERAGE STEP SIZE		0.00000E+00	
DENSITY (G/CM**3)	2.06233E-03			METHOD ORDER		0	
TEMPERATURE (DEG K)	1245.31						
MASS FLUX (G/SEC/CM**2)	3.79704E+01			TOTAL NUMBER OF STEPS		0	
ENTROPY (CAL/G/DEG K)	0.3575			FUNCT EVALUATIONS		0	
MACH NUMBER	0.5098			JACOBIAN EVALUATIONS		0	
GAMMA	1.6577						
ENTHALPY (CAL/G)	3.66089E+01						
SP. HEAT (CP) (CAL/G/DEG K)	3.80671E-02						
CHEMICAL PROPERTIES							
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
BR2	1.56741E-07	1.00000E-02	-3.66694E-05	1	1.4519E+07	8.62161E+00	1.00000
BR	0.00000E+00	0.00000E+00	7.33389E-05				
XE	1.55174E-05	9.90000E-01	0.00000E+00				
DERIVATIVES (CGS UNITS): T							
			5.00570E+00	RHO	1.73397E-05	V	-5.36590E+02
MIXTURE MOLECULAR WEIGHT							
	131.57527		TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	3.97306E+05	MASS FRACTION SUM	1.00000000	
CPU TIME FOR INITIALIZATION OF LSENS = 0.860000 S							
TIME	2.71785E-06	SEC	AREA	1.00125E+00	AXIAL POSITION	5.00000E-02	CM
FLOW PROPERTIES				INTEGRATION INDICATORS			
PRESSURE (ATM)	1.60250			STEPS FROM LAST PRINT		4	
VELOCITY (CM/SEC)	18389.24			AVERAGE STEP SIZE		0.14283E-01	
DENSITY (G/CM**3)	2.06306E-03			METHOD ORDER		1	
TEMPERATURE (DEG K)	1245.51						
MASS FLUX (G/SEC/CM**2)	3.79855E+01			TOTAL NUMBER OF STEPS		4	
ENTROPY (CAL/G/DEG K)	0.3575			FUNCT EVALUATIONS		5	
MACH NUMBER	0.5091			JACOBIAN EVALUATIONS		2	
GAMMA	1.6577						
ENTHALPY (CAL/G)	3.66186E+01						
SP. HEAT (CP) (CAL/G/DEG K)	3.80671E-02						
CHEMICAL PROPERTIES							
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
BR2	1.56697E-07	9.99357E-03	-3.67572E-05	1	1.4553E+07	8.63612E+00	0.99999
BR	1.99794E-10	1.27421E-05	7.35144E-05				
XE	1.55229E-05	9.89994E-01	0.00000E+00				
DERIVATIVES (CGS UNITS): T							
			2.61468E+00	RHO	1.13364E-05	V	-3.30484E+02
MIXTURE MOLECULAR WEIGHT							
	131.57444		TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	3.97974E+05	MASS FRACTION SUM	1.00000000	

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 1.999998E-02 S UP TO THIS TIME - 1.999998E-02 S

TABLE D.2.—Continued.
(a) Concluded.

TIME 2.19540E-04 SEC		AREA 1.01127E+00		AXIAL POSITION 4.00000E+00 CM			
FLOW PROPERTIES				INTEGRATION INDICATORS			
PRESSURE (ATM)		1.61360		STEPS FROM LAST PRINT 2			
VELOCITY (CM/SEC)		18091.43		AVERAGE STEP SIZE 0.14460E+01			
DENSITY (G/CM**3)		2.07827E-03		METHOD ORDER 2			
TEMPERATURE (DEG K)		1244.35					
MASS FLUX (G/SEC/CM**2)		3.80227E+01		TOTAL NUMBER OF STEPS 10			
ENTROPY (CAL/G/DEG K)		0.3576		FUNCT EVALUATIONS 14			
MACH NUMBER		0.5009		JACOBIAN EVALUATIONS 5			
GAMMA		1.6581					
ENTHALPY (CAL/G)		3.67484E+01					
SP. HEAT (CP) (CAL/G/DEG K)		3.80723E-02					
CHEMICAL PROPERTIES							
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
BR2	1.50195E-07	9.50418E-03	-3.32811E-05	1	1.4354E+07	7.70535E+00	0.95156
BR	1.55159E-08	9.81828E-04	6.65621E-05				
XE	1.56374E-05	9.89514E-01	0.00000E+00				
DERIVATIVES (CGS UNITS): T		-5.00701E-01		RHO	3.10388E-06	V	-5.25083E+01
MIXTURE MOLECULAR WEIGHT		131.51068	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)		3.55082E+05	MASS FRACTION SUM	1.00000000
COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 0.000000E+00 S UP TO THIS TIME - 3.000003E-02 S							
(LSENS) END OF THIS CASE							
SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:							
TOTAL NO. OF STEPS -				10			
TOTAL NO. OF DERIVATIVE EVALUATIONS -				14			
TOTAL NO. OF JACOBIAN EVALUATIONS -				5			
TOTAL CPU TIME -				0.031000 S			
TOTAL CPU TIME (INCLUDING I/O) REQUIRED =						1.010000 S	
(LSENS) READ DATA FOR NEXT CASE							

TABLE D.2.—Continued.
(b) Case 2

DISTANCE-AREA VERSION			LHHS SENSITIVITY AND GENERAL KINETICS PROGRAM				NASA LHHS RESEARCH CENTER			
LSEHS			HYDROGEN - AIR TEST WITH HEAT TRANSFER				STOICH		CASE 2	
REACTION NUMBER		REACTION				REACTION RATE VARIABLES		ACTIVATION ENERGY		
						A	B			
1	1*O	+	1*H2O	=	2*OH	6.80000E+13	0.0000	18365.00		
2	1*H	+	1*O2	=	1*OH	1.89000E+14	0.0000	16400.00		
3	1*O	+	1*H2	=	1*OH	4.20000E+14	0.0000	13750.00		
4	1*H	+	1*H2O2	=	1*H2	7.28000E+13	0.0000	2126.00		
5	1*O	+	1*H2O2	=	1*OH	5.00000E+13	0.0000	1000.00		
6	1*H2O2	+	1*OH	=	1*H2O	8.00000E+12	0.0000	0.00		
7	1*H	+	1*H2O2	=	2*OH	1.34000E+14	0.0000	1070.00		
8	1*H2	+	1*H2O2	=	1*H2O2	7.91000E+13	0.0000	25000.00		
9	1*OH	+	1*H2O2	=	1*H2O	6.10000E+12	0.0000	1430.00		
10			2*H2O2	=	1*H2O2	1.80000E+12	0.0000	0.00		
11	1*H	+	1*H2O2	=	1*OH	7.80000E+11	0.0000	0.00		
12	M	+	1*H2O2	=	2*OH	1.44000E+17	0.0000	45510.00		
13	1*H2	+	1*OH	=	1*H2O	4.74000E+13	0.0000	6098.00		
14	1*H	+	1*O2	=	1*H2O	1.46000E+15	0.0000	-1000.00		
15	M	+	1*H2O	=	1*H	1.30000E+15	0.0000	105140.00		
16	1*H	+	1*O	=	1*OH	7.10000E+18	-1.0000	0.00		
17	M	+	1*H2	=	2*H	2.20000E+14	0.0000	96000.00		
18	M	+	1*O2	=	2*O	1.80000E+18	-1.0000	118020.00		
19	1*H2O2	+	1*H2O	=	1*H2O2	2.09000E+12	0.0000	-477.00		
20	1*O	+	1*H2O2	=	1*H2O	1.00000E+13	0.0000	596.00		
21	1*H2O	+	1*O	=	1*H2O2	5.62000E+15	0.0000	-1160.00		
22	1*H2O2	+	1*H	=	1*H2O	3.47000E+14	0.0000	1470.00		
23	1*H2O	+	1*O	=	1*H	3.80000E+09	1.0000	41370.00		
24	1*O	+	1*H2	=	1*H2O	1.80000E+14	0.0000	76250.00		
25	1*H2O	+	1*H	=	1*H	2.65000E+14	0.0000	50410.00		
26	M	+	1*H2O	=	1*H2	6.92000E+23	-2.5000	65000.00		
27	1*O	+	1*H2O	=	1*H2	1.00000E+14	0.0000	28020.00		
28	1*O	+	1*H2O	=	2*H2O	6.92000E+15	0.0000	26630.00		
29	1*H	+	1*H2O2	=	2*H2O	4.00000E+12	0.0000	0.00		
30	1*H2O2	+	1*H	=	1*H2	7.59000E+13	0.0000	15100.00		
31	1*H2O2	+	1*H2	=	1*H2O2	2.40000E+13	0.0000	29000.00		
32	1*OH	+	1*H2O2	=	1*H2O3	3.00000E+15	0.0000	-3800.00		
33	1*OH	+	1*H2O	=	1*H2O2	5.60000E+15	0.0000	-1700.00		
34	1*H2O	+	1*H	=	1*H2	5.00000E+12	0.0000	0.00		
35	1*H	+	1*H2O	=	1*H2O	5.40000E+15	0.0000	-600.00		
36	1*H2O	+	1*OH	=	1*H2O	3.60000E+13	0.0000	0.00		

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	, 12) = 2.30000	M(O2	, 12) = 0.78000	M(H2O	, 12) = 6.00000	M(H2O2	, 12) = 6.60000
M(O2	, 14) = 1.30000	M(H2	, 14) = 1.30000	M(H2O	, 14) = 21.30000	M(H2	, 14) = 3.00000
M(H2	, 15) = 4.00000	M(O2	, 15) = 1.50000	M(H2O	, 15) = 20.00000	M(H2	, 15) = 1.50000
M(H2	, 17) = 4.10000	M(O2	, 17) = 2.00000	M(H2O	, 17) = 15.00000	M(H2	, 17) = 2.00000
M(O2	, 32) = 0.70000	M(H2	, 32) = 1.40000				

** UCH INPUT DATA GIVEN IN CGS UNITS **

** OUTPUT REQUIRED IN CGS UNITS **

** ASSIGNED VARIABLE PROFILE **

THE AREA IS CALCULATED FROM THE FOLLOWING POLYNOMIAL

$$\text{AREA (CM**2)} = (0.00000E+00)X**3 + (0.00000E+00)X**2 + (0.00000E+00)X + (2.00000E+03)$$

THE AREA WILL BE HELD CONSTANT FOR THIS CASE

HEAT TRANSFER CASE: QDOT (CAL/CM-SEC) =

$$(0.00000E+00)T**4 + (0.00000E+00)T**3 + 0.00000E+00T**2 + (5.86300E+00)T + (-4.28800E+01)$$

FUEL-AIR REACTION, FUEL-AIR EQUIVALENCE RATIO = 1.0000 OXYGEN FRACTION IN AIR = 0.2095

NUMBER OF REACTING SPECIES: 16

NUMBER OF INERT SPECIES: 2

NUMBER OF SPECIES ODE'S REQUIRED FOR THIS CASE: 16

TOTAL NUMBER OF ODE'S REQUIRED FOR THIS CASE: 19

INTEGRATION CONTROLS

INTEGRATION METHOD (MF): 21 MAXIMUM RELATIVE ERROR: 5.00000E-03 SPECIES ABSOLUTE ERROR: 1.00000E-12

MAXIMUM NUMBER OF STEPS ALLOWED FOR THE COMPLETE PROBLEM: 2000

** OUTPUT REQUIRED AT FOLLOWING 4 PRINT STATIONS **

STATION	AXIAL DISTANCE (CM)
1	3.04800E+00
2	6.09600E+00
3	7.62000E+00
4	1.21900E+01

TABLE D.2.—Continued
(b) Continued.

** INITIAL CONDITIONS **							
TIME	0.00000E+00	SEC	AREA	2.00000E+03	SQ CM	AXIAL POSITION	0.00000E+00 CM
FLOW PROPERTIES				INTEGRATION INDICATORS			
PRESSURE (ATM)	0.95600		STEPS FROM LAST PRINT	0			
VELOCITY (CM/SEC)	450945.64		AVERAGE STEP SIZE	0.00000E+00			
DENSITY (G/CM**3)	1.56988E-04		METHOD ORDER	0			
TEMPERATURE (DEG K)	1559.00						
MASS FLOW RATE (G/SEC)	1.41586E+05		TOTAL NUMBER OF STEPS	0			
ENTROPY (CAL/G/DEG K)	2.6767		FUNCT EVALUATIONS	0			
MACH NUMBER	5.0000		JACOBIAN EVALUATIONS	0			
GAMMA	1.3183						
ENTHALPY (CAL/G)	4.54652E+02						
SP. HEAT (CP) (CAL/G/DEG K)	3.91820E-01						
HEAT LOSS(QDOT/MDOT) = 6.4254E-02 CAL/(G-CM)							
CHEMICAL PROPERTIES							
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
O	0.00000E+00	0.00000E+00	6.70115E-15	1	1.8115E+11	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	2	9.4932E+11	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	0.00000E+00	3	4.9624E+12	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	1.03759E-05	4	3.6652E+13	4.20984E+02	1.00000
O2	1.10332E-06	1.47639E-01	-1.03755E-05	5	3.6206E+13	0.00000E+00	0.00000
H2	2.20665E-06	2.95278E-01	-1.03756E-05	6	8.0000E+12	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	1.03755E-05	7	9.4865E+13	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	8	2.4747E+10	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	0.00000E+00	9	3.8447E+12	0.00000E+00	0.00000
NO2	0.00000E+00	0.00000E+00	0.00000E+00	10	1.8000E+12	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	0.00000E+00	11	7.8000E+11	0.00000E+00	0.00000
H2	4.11248E-06	5.50505E-01	-1.26958E-15	12	6.0049E+10	0.00000E+00	0.00000
N2O	0.00000E+00	0.00000E+00	1.26958E-15	13	6.6210E+12	0.00000E+00	0.00000
HNH2	0.00000E+00	0.00000E+00	0.00000E+00	14	2.0162E+15	0.00000E+00	0.00000
HNH3	0.00000E+00	0.00000E+00	0.00000E+00	15	2.3703E+00	0.00000E+00	0.00000
HNH	0.00000E+00	0.00000E+00	0.00000E+00	16	4.5542E+15	0.00000E+00	0.00000
CO2	1.57996E-09	2.11419E-04	0.00000E+00	17	7.6662E+00	1.34051E-02	1.00000
AR	4.90836E-05	6.56802E-03	0.00000E+00	18	3.2937E-02	1.10195E-05	1.00000
				19	2.4379E+12	0.00000E+00	0.00000
				20	8.2499E+12	0.00000E+00	0.00000
				21	8.1724E+15	0.00000E+00	0.00000
				22	2.1590E+14	0.00000E+00	0.00000
				23	9.4003E+06	0.00000E+00	0.00000
				24	3.6821E+03	0.00000E+00	0.00000
				25	2.2552E+07	0.00000E+00	0.00000
				26	5.5707E+06	0.00000E+00	0.00000
				27	1.1803E+10	-5.15143E-06	1.00000
				28	1.2793E+10	0.00000E+00	0.00000
				29	4.0000E+12	0.00000E+00	0.00000
				30	5.8001E+11	0.00000E+00	0.00000
				31	2.0645E+09	0.00000E+00	0.00000
				32	1.0229E+16	0.00000E+00	0.00000
				33	9.6940E+15	0.00000E+00	0.00000
				34	5.0000E+12	0.00000E+00	0.00000
				35	6.5540E+15	0.00000E+00	0.00000
				36	3.1000E+13	0.00000E+00	0.00000
DERIVATIVES (CGS UNITS): T -2.44902E-01 RHO -7.71706E-10 V 2.21672E+00							
MIXTURE MOLECULAR WEIGHT 21.00704 TOTAL ENERGY EXCHANGE RATE 2.21461E+07 MASS FRACTION SUM 1.00000000							
(CAL-CM**3/G**2/SEC)							
CPU TIME FOR INITIALIZATION OF LSENS = 1.210000 S							

TABLE D.2.—Continued.
(b) Continued.

TIME	1.35672E-05	SEC	AREA	2.00000E+03	SQ CM	AXIAL POSITION	6.09600E+00	CM
FLOW PROPERTIES				INTEGRATION INDICATORS				
PRESSURE (ATM)	1.32771		STEPS FROM LAST PRINT		27			
VELOCITY (CM/SEC)	445625.60		AVERAGE STEP SIZE		0.15164E+00			
DENSITY (G/CM**3)	1.58862E-04		METHOD ORDER		3			
TEMPERATURE (DEG K)	2217.16		TOTAL NUMBER OF STEPS		72			
MASS FLOW RATE (G/SEC)	1.41586E+05		FUNCT EVALUATIONS		107			
ENTROPY (CAL/G/DEG K)	2.7814		JACOBIAN EVALUATIONS		18			
MACH NUMBER	4.2705							
GAMMA	1.2858							
ENTHALPY (CAL/G)	5.11217E+02							
SP. HEAT (CP) (CAL/G/DEG K)	4.10646E-01							
HEAT LOSS(QDOT/MDOT) = 9.1509E-02 CAL/(G-CM)								
CHEMICAL PROPERTIES								
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONSL COS UNITS	NET REACTION CONV RATE (MOLE (CM**3/G**2/SEC))	NET RATE/POSTIVE DIR RATE	
O	2.00774E-07	2.75114E-02	-6.77700E-03	1	1.0525E+12	5.09436E+03	0.00046	
H2O	1.32763E-06	1.81922E-01	1.27487E-02	2	4.5697E+12	7.50542E+04	0.00298	
OH	2.39442E-07	3.28100E-02	8.54901E-03	3	1.8531E+13	1.93022E+05	0.00269	
H	5.98048E-07	8.19487E-02	-3.43219E-02	4	4.4933E+13	1.11542E+05	0.96560	
O2	2.32416E-07	3.18473E-02	-7.25712E-03	5	3.9847E+13	3.52109E+04	0.96569	
H2	4.86522E-07	6.66466E-02	1.43512E-04	6	8.0000E+12	7.25148E+03	0.96568	
H2O2	1.08487E-10	1.48656E-05	-4.01910E-06	7	1.0511E+14	2.60970E+05	0.96580	
H2O2	3.89387E-11	5.33566E-06	-3.79636E-06	8	2.7157E+11	-6.62640E+04	0.98787	
H2O	1.59973E-11	2.19206E-06	9.07028E-06	9	4.4073E+12	1.60926E+03	0.98790	
H2O2	1.35782E-15	1.86058E-10	7.77293E-10	10	1.8000E+12	-1.54158E+00	0.64745	
H	3.32450E-13	4.56232E-08	1.19583E-07	11	7.8000E+11	7.19435E+02	0.99959	
H2	4.16156E-06	5.70247E-01	-6.63857E-06	12	4.7029E+12	-4.84438E+04	0.31501	
H2O	5.75396E-13	7.88448E-08	3.68849E-08	13	1.1876E+13	1.22471E+05	0.00273	
H2O2	2.12750E-15	2.91525E-10	1.03301E-09	14	1.8320E+15	3.65639E+05	0.99174	
H2O3	3.23871E-20	4.43791E-15	-6.22870E-14	15	5.6249E+04	-3.77492E+05	0.99972	
H2O	2.67768E-14	3.66915E-09	1.16987E-08	16	3.2023E+15	1.11156E+05	0.99977	
CO2	1.59882E-09	2.19082E-04	0.00000E+00	17	7.5777E+04	-1.63370E+05	0.99912	
AK	4.96696E-08	6.80607E-03	0.00000E+00	18	1.8882E+03	4.46331E+02	0.99972	
				19	2.5290E+12	1.11339E+01	0.69518	
				20	8.7348E+12	8.37547E-02	0.88745	
				21	7.3127E+15	6.77466E+00	0.99747	
				22	2.4856E+14	7.10025E+00	0.88779	
				23	7.0416E+08	-1.56957E+01	0.99150	
				24	5.4850E+06	1.81586E+02	0.99996	
				25	2.8246E+09	-1.63152E+02	0.99348	
				26	1.1707E+09	-3.48602E+01	0.99444	
				27	1.7299E+11	7.51363E+01	0.94885	
				28	1.6411E+11	7.51231E+01	1.00000	
				29	4.0000E+12	7.16014E+08	0.99927	
				30	2.4650E+12	3.18961E+01	0.94900	
				31	3.5238E+10	-3.28787E+01	0.99736	
				32	7.1071E+15	-2.46807E-06	0.00362	
				33	8.2368E+15	3.69719E-01	0.04052	
				34	5.0000E+12	3.16912E+00	0.99888	
				35	6.1878E+15	1.27682E+01	0.74586	
				36	3.6000E+13	9.13558E+00	0.99888	
DERIVATIVES (COS UNITS), T	1.27427E+02		RHO	5.48122E-07	V	-9.76519E+02		
MIXTURE MOLECULAR WEIGHT	21.76841		TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	-1.12877E+11		MASS FRACTION SUM	1.00000031	

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 4.500000E-01 S UP TO THIS TIME - 1.110000E+00 S

TABLE D.2.—Continued.
(b) Concluded.

TIME	2.73051E-05	SEC	AREA	2.00000E+03	SQ CM	AXIAL POSITION	1.21900E+01	CM
FLOW PROPERTIES				INTEGRATION INDICATORS				
PRESSURE (ATM)	1.57011			STEPS FROM LAST PRINT			8	
VELOCITY (CM/SEC)	442156.36			AVERAGE STEP SIZE			0.60182E+00	
DENSITY (G/CM**3)	1.60109E-04			METHOD ORDER			2	
TEMPERATURE (DEG K)	2683.01							
MASS FLOW RATE (G/SEC)	1.41586E+05			TOTAL NUMBER OF STEPS			82	
ENTROPY (CAL/G/DEG K)	2.7965			FUNCT EVALUATIONS			128	
MACH NUMBER	3.9384			JACOBIAN EVALUATIONS			21	
GAMMA	1.2685							
ENTHALPY (CAL/G)	5.47385E+02							
SP. HEAT (CP) (CAL/G/DEG K)	4.18231E-01							
HEAT LOSS(QDOT/MDOT) = 1.1080E-01 CAL/(G-CM)								
CHEMICAL PROPERTIES								
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST (CGS UNITS)	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE	
O	1.57445E-07	1.92722E-02	-3.20044E-03	1	2.1705E+12	-6.55786E+03	0.00058	
H2O	1.46834E-06	2.05888E-01	7.35139E-03	2	8.7211E+12	7.20425E+03	0.00054	
OH	2.87650E-07	4.03336E-02	4.53908E-04	3	3.1858E+13	8.78750E+04	0.00111	
H	3.51216E-07	4.92467E-02	-9.33410E-03	4	4.8860E+13	4.21963E+04	0.61722	
O2	1.78006E-07	2.48596E-02	-2.37435E-03	5	4.1449E+13	1.40180E+04	0.61765	
H2	4.62674E-07	4.48751E-02	-2.91830E-03	6	8.1000E+12	5.66374E+03	0.61780	
HO2	1.02125E-10	1.43198E-05	2.51558E-06	7	1.1963E+14	9.47669E+04	0.61778	
H2O2	1.25021E-11	1.75301E-06	5.72723E-06	8	7.7737E+11	-8.90178E+03	0.86410	
HO	8.32965E-10	1.16796E-04	1.27179E-04	9	4.6649E+12	5.68895E+02	0.86930	
N	1.15525E-13	1.61987E-08	1.75775E-08	10	1.8000E+12	-1.40920E+00	0.65803	
N2	3.80501E-12	5.33530E-07	3.73859E-07	11	7.8000E+11	1.26950E+02	0.95004	
HNO2	4.19380E-06	5.88046E-01	-6.39038E-05	12	2.8266E+13	-9.82245E+03	0.04524	
N2O	1.44988E-12	2.03299E-07	1.03762E-07	13	1.5103E+13	1.17251E+05	0.00150	
HNO	2.52785E-14	3.54450E-09	3.44329E-09	14	1.7612E+15	1.47272E+05	0.87521	
HNO3	6.38880E-19	8.95824E-14	9.63872E-13	15	3.5447E+06	-1.56494E+05	0.95230	
HO	3.51863E-13	4.93374E-08	2.65498E-08	16	2.6463E+15	3.38432E+04	0.95229	
CO2	1.61137E-09	2.25942E-04	0.00000E+00	17	5.5310E+06	-6.01419E+04	0.95223	
AR	5.00593E-08	7.01920E-03	0.00000E+00	18	1.4335E+05	-1.61391E+02	0.95227	
				19	2.2856E+12	1.94616E+00	0.25659	
				20	8.5426E+12	2.69015E+00	0.48568	
				21	6.5860E+15	2.01860E+02	0.90720	
				22	2.6338E+14	2.02541E+02	0.48585	
				23	4.1505E+09	-1.88729E+02	0.90666	
				24	1.1071E+08	2.68517E+05	0.99829	
				25	2.6595E+10	-2.28186E+03	0.90663	
				26	9.4158E+09	-4.45600E+01	0.92113	
				27	5.2189E+11	1.60165E+00	0.39478	
				28	4.6372E+11	3.64335E+00	0.99990	
				29	4.0300E+12	6.52974E-05	0.95199	
				30	4.4595E+12	5.50673E+01	0.99668	
				31	1.0422E+11	-2.11147E+00	0.00065	
				32	6.1187E+15	3.76002E-05	0.00457	
				33	7.7031E+15	2.24581E+00	0.93011	
				34	5.0000E+12	2.24193E+01	0.93011	
				35	6.0432E+15	1.55674E+02	0.93022	
				36	5.6000E+13	1.32219E+02	0.93022	
DERIVATIVES (CGS UNITS): T	4.69727E+01		RHO	1.25045E-07	V	-3.39801E+02		
MIXTURE MOLECULAR WEIGHT	22.45008	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)		-4.27131E+10	MASS FRACTION SUM		1.00000020	
COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 1.80000E-01 S UP TO THIS TIME - 1.31000E+00 S								
(LENS) END OF THIS CASE								
SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:								
TOTAL NO. OF STEPS - 82								
TOTAL NO. OF DERIVATIVE EVALUATIONS - 128								
TOTAL NO. OF JACOBIAN EVALUATIONS - 21								
TOTAL CPU TIME - 1.310000 S								
TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 5.110000 S								
(LENS) READ DATA FOR NEXT CASE								

TABLE D.2.—Continued.
(c) Case 3

DISTANCE-AREA VERSION		LEHS SENSITIVITY AND GENERAL KINETICS PROGRAM		NASA LEHS RESEARCH CENTER	
LSEHS		HYDROGEN - AIR TEST WITH HEAT TRANSFER		FULL MECHANISM	
CASE 3					
REACTION NUMBER	REACTION		REACTION RATE VARIABLES		ACTIVATION ENERGY
1	1*H	+ 1*H2O	= 2*OH	+ 1*H	18565.00
2	1*H	+ 1*O2	= 1*OH	+ 1*H	14500.00
3	1*H	+ 1*H2	= 1*H2	+ 1*H	13750.00
4	1*H	+ 1*H2O	= 1*H2	+ 1*O2	2126.00
5	1*H	+ 1*H2O	= 1*H2	+ 1*O2	1000.00
6	1*H2O	+ 1*OH	= 1*H2O	+ 1*O2	0.0000
7	1*H	+ 1*H2O	= 2*OH		1070.00
8	1*H2	+ 1*H2O	= 1*H2O2	+ 1*H	25000.00
9	1*OH	+ 1*H2O2	= 1*H2O	+ 1*H2O	1430.00
10	1*H	+ 1*H2O2	= 1*OH	+ 1*H2O	0.0000
11	1*H	+ 1*H2O2	= 2*OH		0.0000
12	1*H	+ 1*H2O2	= 2*OH		45510.00
13	1*H2	+ 1*OH	= 1*H2O	+ 1*H	6090.00
14	1*H	+ 1*O2	= 1*H2	+ 1*H	1000.00
15	1*H	+ 1*H2O	= 1*H	+ 1*OH	105140.00
16	1*H	+ 1*O	= 1*OH	+ 1*H	0.0000
17	1*H	+ 1*H2	= 2*H		96000.00
18	1*H	+ 1*O2	= 2*H		118020.00
19	1*H2O	+ 1*H2O	= 1*H2O	+ 1*OH	-477.00
20	1*H	+ 1*H2O2	= 1*H2O	+ 1*O2	596.00
21	1*H2O	+ 1*H	= 1*H2O	+ 1*H	-1160.00
22	1*H2O	+ 1*H	= 1*H2O	+ 1*OH	1470.00
23	1*H2	+ 1*H	= 1*H	+ 1*O2	41370.00
24	1*H	+ 1*H2	= 1*H2	+ 1*H	76250.00
25	1*H2	+ 1*H	= 1*H	+ 1*OH	50410.00
26	1*H2	+ 1*H2O	= 1*H2	+ 1*O2	45000.00
27	1*H	+ 1*H2O	= 1*H2	+ 1*O2	28020.00
28	1*H	+ 1*H2O	= 2*H2		26630.00
29	1*H	+ 1*H2O	= 2*H2		0.0000
30	1*H2O	+ 1*H	= 1*H2	+ 1*OH	15100.00
31	1*H2O	+ 1*H2	= 1*H2O2	+ 1*H	29000.00
32	1*OH	+ 1*H2O	= 1*H2O	+ 1*H	-3800.00
33	1*OH	+ 1*H2O	= 1*H2O	+ 1*H	-1700.00
34	1*H2O	+ 1*H	= 1*H2	+ 1*H2O	0.0000
35	1*H	+ 1*H2O	= 1*H2O	+ 1*H	-600.00
36	1*H2O	+ 1*OH	= 1*H2O	+ 1*H2O	0.0000
37	1*H	+ 1*H2O2	= 1*OH	+ 1*H2O	1000.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	, 12) = 2.30000	M(O2	, 12) = 0.78000	M(H2O	, 12) = 6.00000	M(H2O2	, 12) = 6.60000
M(O2	, 14) = 1.30000	M(H2	, 14) = 1.30000	M(H2O	, 14) = 21.30000	M(H2	, 14) = 3.00000
M(H2	, 15) = 4.00000	M(O2	, 15) = 1.50000	M(H2O	, 15) = 20.00000	M(H2	, 15) = 1.50000
M(H2	, 17) = 4.10000	M(O2	, 17) = 2.00000	M(H2O	, 17) = 15.00000	M(H2	, 17) = 2.00000
M(O2	, 32) = 0.70000	M(H2	, 32) = 1.40000				

== INITIAL CONDITIONS ==

TIME 0.00000E+00 SEC AREA 2.00000E+03 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE 0.95600
(ATM)
VELOCITY 450950.60
(CM/SEC)
DENSITY 1.56985E-04
(G/CM**3)
TEMPERATURE 1559.00
(DEG K)
MASS FLOW RATE 1.41585E+05
(G/SEC)
ENTROPY 2.6768
(CAL/G-DEG K)
MACH NUMBER 5.0000
QAMMA 1.5185
ENTHALPY 4.56661E+02
(CAL/G)
SP. HEAT (CP) 3.91828E-01
(CAL/G-DEG K)

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 0
AVERAGE STEP SIZE 0.00000E+00
METHOD ORDER 0
TOTAL NUMBER OF STEPS 0
FUNC EVALUATIONS 0
JACOBIAN EVALUATIONS 0

HEAT LOSS(QDOT/MDOT) = 6.4255E-02 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3-SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	NET WALL/POST- TIVE DIR RATE
O	0.00000E+00	0.00000E+00	6.70095E-15	1	1.8113E+11	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	2	9.4932E+11	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	0.00000E+00	3	4.9624E+12	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	1.03765E-05	4	3.6652E+13	2.2144E+07	1.00000
O2	1.10330E-06	1.47636E-01	-1.03756E-05	5	3.6206E+13	0.00000E+00	0.00000
H2	2.20678E-06	2.95295E-01	-1.03760E-05	6	8.0000E+12	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	1.03756E-05	7	9.4865E+13	0.00000E+00	0.00000
HO	0.00000E+00	0.00000E+00	0.00000E+00	8	2.4747E+10	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	0.00000E+00	9	3.8447E+12	0.00000E+00	0.00000
N	0.00000E+00	0.00000E+00	0.00000E+00	10	2.0000E+12	0.00000E+00	0.00000
N2	4.11238E-06	5.50290E-01	-1.26952E-13	11	7.8000E+11	0.00000E+00	0.00000
N2O	0.00000E+00	0.00000E+00	0.00000E+00	12	6.0049E+10	0.00000E+00	0.00000
HN2O	0.00000E+00	0.00000E+00	0.00000E+00	13	6.6210E+12	0.00000E+00	0.00000
HN2O2	0.00000E+00	0.00000E+00	0.00000E+00	14	2.0162E+15	0.00000E+00	0.00000
HN2O3	0.00000E+00	0.00000E+00	0.00000E+00	15	2.3703E+00	0.00000E+00	0.00000
HN2O	0.00000E+00	0.00000E+00	0.00000E+00	16	4.5542E+15	0.00000E+00	0.00000
CO2	1.57992E-09	2.11414E-04	0.00000E+00	17	7.6682E+00	1.39704E+03	1.00000
AR	4.90825E-08	6.56787E-03	0.00000E+00	18	3.2937E-02	1.31255E+00	1.00000
				19	2.4579E+12	0.00000E+00	0.00000
				20	8.2499E+12	0.00000E+00	0.00000
				21	8.1724E+15	0.00000E+00	0.00000
				22	2.1590E+14	0.00000E+00	0.00000
				23	9.4003E+06	0.00000E+00	0.00000
				24	5.0821E+03	0.00000E+00	0.00000
				25	2.552E+07	0.00000E+00	0.00000
				26	5.5707E+06	0.00000E+00	0.00000
				27	1.1803E+10	4.07252E-01	1.00000
				28	1.2793E+10	0.00000E+00	0.00000
				29	4.0000E+12	0.00000E+00	0.00000
				30	5.8001E+11	0.00000E+00	0.00000
				31	2.0645E+09	0.00000E+00	0.00000
				32	1.0229E+16	0.00000E+00	0.00000
				33	9.6940E+15	0.00000E+00	0.00000
				34	5.0000E+12	0.00000E+00	0.00000
				35	6.5540E+15	0.00000E+00	0.00000
				36	3.6000E+13	0.00000E+00	0.00000
				37	5.7930E+13	0.00000E+00	0.00000

DERIVATIVES (CGS UNITS): T -2.44900E-01 RHO -7.71685E-10 V 2.21672E+00
MIXTURE MOLECULAR WEIGHT 21.00658 TOTAL ENERGY EXCHANGE RATE 2.21478E+07 MASS FRACTION SUM 1.00000000

CPU TIME FOR INITIALIZATION OF LSEHS = 0.580000 S

TABLE D.2.—Continued.
(c) Continued.

TIME	1.35672E-05	SEC	AREA	2.00000E+05	SQ CM	AXIAL POSITION	6.09600E+00	CM
FLOW PROPERTIES				INTEGRATION INDICATORS				
PRESSURE (ATM)	1.32893		STEPS FROM LAST PRINT		25			
VELOCITY (CM/SEC)	445612.90		AVRAGL STEP SIZE		0.12184E+00			
DENSITY (G/CM**3)	1.50865E-04		METHOD UNDER		5			
TEMPERATURE (DEG K)	2219.44		TOTAL NUMBER OF STEPS		70			
MASS FLOW RATE (G/SEC)	1.41585E+05		FUNCT EVALUATIONS		109			
ENTROPY (CAL/G/DEG K)	2.7816		JACOBIAN EVALUATIONS		19			
MACH NUMBER	4.2686							
GAMMA	1.2858							
ENTHALPY (CAL/G)	5.11414E+02							
SP. HEAT (CP) (CAL/G/DEG K)	4.10698E-01							
HEAT LOSS(QDOT/MDOT) = 9.1604E-02 CAL/(G-CM)								
CHEMICAL PROPERTIES								
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE	
O	2.00450E-07	2.74700E-01	-6.52579E-05	1	1.0571E+12	4.25857E+07	0.00023	
H2O	1.32820E-06	1.82018E-01	1.28361E-02	2	4.5872E+12	1.44486E+09	0.00542	
OH	2.39788E-07	3.28609E-02	8.50641E-05	3	1.8590E+13	5.34580E+08	0.00249	
H	5.96769E-07	8.17821E-02	-3.48516E-02	4	4.4956E+13	-6.01256E+09	0.96601	
O2	2.32143E-07	3.18135E-02	-7.40807E-05	5	1.9857E+13	-1.72713E+09	0.96609	
H2	4.86645E-07	6.66906E-02	3.19165E-04	6	4.0000E+12	-5.52641E+08	0.96609	
H2O2	1.11512E-10	1.52544E-05	-4.02841E-06	7	1.0513E+14	-9.08151E+09	0.96621	
H2O2	3.44419E-11	4.71997E-06	-9.09783E-07	8	2.7316E+11	-7.75899E+08	0.98583	
H2O	1.62578E-11	2.22800E-06	9.21933E-06	9	4.108E+12	-4.84265E+07	0.98586	
H2O	1.58234E-15	1.89438E-10	6.93502E-10	10	2.0000E+12	4.61206E+04	0.58115	
H	3.37749E-13	4.62856E-08	1.20388E-07	11	7.8000E+11	-4.31744E+07	0.99952	
H2	4.16165E-06	5.70317E-01	-4.71390E-06	12	4.7550E+12	5.07344E+09	0.58919	
H2O	5.76245E-13	7.89695E-08	3.74619E-08	13	1.1893E+13	-1.87286E+09	0.00227	
H2O2	2.16756E-15	2.94305E-10	6.82685E-10	14	1.8516E+15	-1.87997E+10	0.99140	
H2O3	3.25591E-20	4.46195E-15	9.58168E-15	15	5.7642E+04	-4.48379E+10	0.99971	
H2O	2.70663E-14	3.70921E-09	1.17877E-08	16	5.1990E+15	-1.11196E+10	0.99971	
CO2	1.59854E-09	2.19109E-04	0.00000E+00	17	7.7490E+04	-1.69212E+10	0.99971	
AR	4.96704E-08	6.80691E-03	0.00000E+00	18	1.938E+05	5.29303E+07	0.99971	
				19	2.3287E+12	-5.65088E+02	0.70169	
				20	9.7360E+12	-5.90309E+03	0.88634	
				21	7.3108E+15	5.02902E+05	0.99742	
				22	2.4866E+14	-2.10028E+05	0.88675	
				23	7.1170E+08	-4.40001E+05	0.99344	
				24	5.5833E+06	1.38833E+07	0.99996	
				25	2.8579E+09	-8.02522E+06	0.99542	
				26	1.1855E+09	-1.39982E+06	0.99438	
				27	1.7412E+11	-5.97188E+04	0.96791	
				28	1.6513E+11	-2.67780E+04	1.00000	
				29	4.0000E+12	5.73204E-03	0.99925	
				30	2.4736E+12	-1.99039E+06	0.94809	
				31	5.3663E+10	-8.36023E+05	0.99731	
				32	7.1008E+15	-1.87912E-02	0.00055	
				33	1.2336E+15	-1.78713E+04	0.03861	
				34	5.0000E+12	-1.76761E+05	0.99886	
				35	1.8649E+15	-6.39455E+05	0.76389	
				36	5.6000E+13	-6.44390E+05	0.99886	
				37	1.5770E+13	-2.95047E+08	0.98587	
DERIVATIVES (CGS UNITS): I	1.28222E+02		RHO	5.50186E-07	V	-9.82264E+02		
MIXTURE MOLECULAR WEIGHT	21.7713		TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	-1.15492E+11		MASS FRACTION SUM	1.00000051	
COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP = 4.900002E-01 S UP TO THIS TIME = 1.150000E+00 S								

TABLE D.2.—Continued.
(c) Concluded.

TIME	2.73102E-05	SEC	AREA	2.00000E+03	SQ CM	AXIAL POSITION	1.21920E+01	CM
FLOW PROPERTIES					INTEGRATION INDICATORS			
PRESSURE (ATM)	1.57184				STEPS FROM LAST PRINT	7		
VELOCITY (CM/SEC)	442136.92				AVERAGE STEP SIZE	0.66052E+00		
DENSITY (G/CM**3)	1.60114E-04				METHOD ORDER	2		
TEMPERATURE (DEG K)	2686.45				TOTAL NUMBER OF STEPS	81		
MASS FLOW RATE (G/SEC)	1.41585E+03				FNCT EVALUATIONS	129		
ENTROPY (CAL/G/DEG K)	2.7966				JACOBIAN EVALUATIONS	22		
MACH NUMBER	3.9563							
GAMMA	1.2683							
ENTHALPY (CAL/G)	5.47634E+02							
SP. HEAT (CP) (CAL/G/DEG K)	4.18288E-01							
HEAT LOSS(QDOT/MDOT) = 1.1094E-01 CAL/(G-CM)								
CHEMICAL PROPERTIES								
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST COS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	HLI RATE/POSTIVE DIR RATE	
O	1.36917E-07	1.92016E-02	-3.09906E-03	1	2.1801E+12	-9.25500E+07	0.00032	
H2O	1.46965E-06	2.06108E-01	7.05653E-03	2	8.7555E+12	1.88803E+08	0.00033	
OH	2.87774E-07	4.03582E-02	7.69777E-04	3	3.1963E+13	1.55573E+08	0.00106	
H	3.49652E-07	4.90362E-02	-9.71057E-03	4	4.8885E+13	-2.24489E+09	0.61744	
O2	1.77582E-07	2.49046E-02	-2.41684E-03	5	4.1459E+13	-7.19535E+08	0.61785	
H2	4.62362E-07	6.48400E-02	-2.57415E-03	6	8.0000E+12	-3.88369E+08	0.61797	
H2O2	1.03667E-10	1.45386E-05	1.19174E-06	7	1.0966E+14	3.25502E+09	0.61805	
HO	1.22152E-11	1.71509E-06	-1.25994E-05	8	7.3175E+11	-1.63667E+08	0.86281	
H2O2	8.47280E-10	1.18825E-04	1.29050E-04	9	4.6665E+12	-1.87927E+07	0.86300	
HO2	1.18107E-13	1.65636E-08	2.20897E-08	10	2.0000E+12	5.03511E+04	0.64138	
N	3.86102E-12	5.41480E-07	5.50739E-07	11	7.8000E+11	-8.37399E+06	0.96767	
N2	4.19394E-06	5.88169E-01	-6.48330E-05	12	2.8576E+13	-6.41412E+08	0.05763	
N2O	1.46727E-12	2.05774E-07	1.03628E-07	13	1.5125E+13	-1.62137E+09	0.00138	
N2O2	2.56416E-14	3.57080E-09	6.07427E-09	14	1.7608E+15	-7.51326E+09	0.87092	
HNH3	6.47257E-19	9.07731E-14	5.57453E-13	15	3.6555E+06	-1.85008E+10	0.95069	
HHO	3.53811E-13	4.96195E-08	2.96754E-08	16	2.6429E+15	-3.42577E+09	0.95067	
CO2	1.61162E-09	2.25990E-04	0.00000E+00	17	3.4086E+06	-4.13239E+09	0.95062	
AR	5.00607E-08	7.02068E-03	0.00000E+00	18	1.6783E+05	-1.90176E+07	0.95065	
				19	2.2853E+12	-9.92867E+03	0.26292	
				20	8.9436E+12	-1.24722E+05	0.48153	
				21	6.9840E+15	-1.49241E+07	0.90481	
				22	2.4348E+14	-5.9593E+06	0.48181	
				23	4.3996E+09	-6.05406E+06	0.90584	
				24	1.1276E+08	1.89677E+08	0.99826	
				25	2.0844E+10	-1.12041E+08	0.90579	
				26	9.5333E+09	-1.77348E+06	0.91973	
				27	5.2541E+11	-1.26592E+05	0.38892	
				28	4.7172E+11	-1.30961E+05	0.99900	
				29	4.0000E+12	-5.24440E+00	0.95118	
				30	4.4856E+12	-2.17636E+06	0.38924	
				31	1.0495E+11	-5.3173E+04	0.90428	
				32	6.1131E+15	-1.07625E+00	0.00037	
				33	7.6999E+15	-1.17156E+05	0.00450	
				34	5.0000E+12	-1.22427E+06	0.92803	
				35	6.0423E+15	-7.73907E+06	0.33383	
				36	3.6000E+13	-9.24737E+06	0.92813	
				37	6.6334E+13	-6.40678E+07	0.86295	
DERIVATIVES (COS UNITS): T			4.66737E+01	RHO	1.22124E-07	V	-5.37231E+02	
MIXTURE MOLECULAR HEIGHT			22.45486	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)		-4.24354E+10	MASS FRACTION SUM	1.0000000
COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP = 1.500001E-01 S UP TO THIS TIME = 1.360001E+00 S								
(LSLHS) END OF THIS CASE								
SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:								
TOTAL NO. OF STEPS =			81					
TOTAL NO. OF DERIVATIVE EVALUATIONS =			129					
TOTAL NO. OF JACOBIAN EVALUATIONS =			22					
TOTAL CPU TIME =			1.360001 S					
TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 2.500000 S								
(LSRHS) READ DATA FOR NEXT CASE								

TABLE D.2.—Continued
(d) Case 4.

DISTANCE-PRESSURE VERSION LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

LEWIS HYDROGEN - OXYGEN CASE WITH HEAT TRANSFER

CASE 4

REACTION NUMBER	REACTION				REACTION RATE VARIABLES		ACTIVATION ENERGY
					A	N	
1	1*O	+	1*H2O	=	2*OH	0.0000	18365.00
2	1*H	+	1*O2	=	1*OH	0.0000	16400.00
3	1*O	+	1*H2	=	1*OH	0.0000	13750.00
4	1*H	+	1*H2	=	1*H2	0.0000	2126.00
5	1*O	+	1*H2	=	1*OH	0.0000	1000.00
6	1*H2O	+	1*OH	=	1*H2O	0.0000	0.00
7	1*H	+	1*H2	=	2*OH	0.0000	1070.00
8	1*H2	+	1*H2	=	1*H2O2	0.0000	25000.00
9	1*OH	+	1*H2O2	=	1*H2O	0.0000	1430.00
10			2*H2O2	=	1*H2O2	0.0000	0.00
11	1*H	+	1*H2O2	=	1*OH	0.0000	0.00
12	M	+	1*H2O2	=	2*OH	0.0000	45510.00
13	1*H2	+	1*OH	=	1*H2O	0.0000	6098.00
14	1*H	+	1*O2	=	1*H2	0.0000	-1000.00
15	M	+	1*H2O	=	1*H	0.0000	105140.00
16	1*H	+	1*O	=	1*OH	-1.0000	0.00
17	M	+	1*H2	=	2*H	0.0000	96000.00
18	M	+	1*O2	=	2*O	-1.0000	118020.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	, 12) =	2.30000	M(O2	, 12) =	0.78000	M(H2O	, 12) =	6.00000	M(H2O2	, 12) =	6.60000
M(O2	, 14) =	1.30000	M(H2	, 14) =	3.00000	M(H2O	, 14) =	21.30000	M(H2	, 15) =	4.00000
M(O2	, 15) =	1.50000	M(H2O	, 15) =	20.00000	M(H2	, 17) =	4.10000	M(O2	, 17) =	2.00000
M(H2O	, 17) =	15.00000									

** INITIAL CONDITIONS **

TIME	0.00000E+00	SEC	AREA	2.15280E+00	SQ FT	AXIAL POSITION	0.00000E+00	FT
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FLOW PROPERTIES

PRESSURE (LB/FT**2)	1.05810E+04
VELOCITY (FT/SEC)	1.62598E+03
DENSITY (LB/FT**3)	4.35122E-02
TEMPERATURE (DEG R)	1890.00
MASS FLOW RATE (LB/SEC)	1.52297E+02
ENTROPY (BTU/LB/DEG R)	3.68867E+00
MACH NUMBER	5.00000E-01
GAMMA	1.35148E+00
ENTHALPY (BTU/LB)	8.22027E+02
SP. HEAT (CP) (BTU/LB/DEG R)	6.36196E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

HEAT LOSS(QDOT/MDOT) = 4.8552E+00 BTU/(LB-FT)

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/FT**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/FT**3/SEC)	REACTION NUMBER	RATE CONST COS UNITS	NET REACTION CONV RATE (MOLE-FT**3/LB**2/SEC)	NET RATE/POSI- TIVE DIR RATE
O	0.00000E+00	0.00000E+00	6.54229E-17	1	1.0232E+10	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	2	7.2933E+10	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	0.00000E+00	3	5.7715E+11	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	3.55695E-05	4	2.6280E+13	-1.87869E-02	0.00000
O2	1.20765E-03	3.3333E-01	-3.55695E-05	5	3.0962E+13	0.00000E+00	0.00000
H2	2.41531E-03	6.6667E-01	-3.55695E-05	6	8.0000E+12	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	3.55695E-05	7	8.0240E+13	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	8	4.9501E+08	0.00000E+00	0.00000
				9	3.0739E+12	0.00000E+00	0.00000
				10	1.8000E+12	0.00000E+00	0.00000
				11	7.8000E+11	0.00000E+00	0.00000
				12	4.8505E+07	0.00000E+00	0.00000
				13	2.5499E+12	0.00000E+00	0.00000
				14	2.3577E+15	0.00000E+00	0.00000
				15	1.6976E-07	0.00000E+00	0.00000
				16	6.7619E+15	0.00000E+00	0.00000
				17	2.2947E-06	5.77599E-10	1.00000
				18	4.6675E-10	1.72773E-14	1.00000

DERIVATIVES (FPS UNITS): T	2.22574E+01	RHO	2.14009E-03	V	-2.93352E+02
MIXTURE MOLECULAR WEIGHT	12.01013	TOTAL ENERGY EXCHANGE RATE	1.77867E+03	MASS FRACTION SUM	1.00000000

(BTU-FT**3/LB**2/SEC)

CPU TIME FOR INITIALIZATION OF LSENS = 0.900000 S

TABLE D.2.—Continued.
(d) Continued.

TIME	2.08104E-04	SEC	AREA	2.25905E+00	SQ FT	AXIAL POSITION	3.28100E-01	FT
FLOW PROPERTIES			INTEGRATION INDICATORS					
PRESSURE (LB/FT**2)	1.07926E+04		STEPS FROM LAST PRINT			101		
VELOCITY (FT/SEC)	1.52749E+03		AVERAGE STEP SIZE			0.99075E-01		
DENSITY (LB/FT**3)	4.41395E-02		METHOD ORDER			2		
TEMPERATURE (DEG R)	1900.90							
MASS FLOW RATE (LB/SEC)	1.52297E+02		TOTAL NUMBER OF STEPS			101		
ENTROPY (BTU/LB/DEG R)	3.68915E+00		FUNCT EVALUATIONS			129		
MACH NUMBER	4.68508E-01		JACOBIAN EVALUATIONS			17		
GAMMA	1.35101E+00							
ENTHALPY (BTU/LB)	8.26637E+02							
SP. HEAT (CP) (BTU/LB/DEG R)	6.36664E-01							
HEAT LOSS(QDOT/MDOT) = 4.8834E+00 BTU/(LB-FT)								
CHEMICAL PROPERTIES								
SPECIES	CONCENTRATION (MOLES/FT**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/FT**3/SEC)	REACTION NUMBER	RATE CONST COS UNITS	NET REACTION CONV RATE (MOLE-FT**3/LB**2/SEC)	NET RATE/POSI- TIVE DIR RATE	
O	2.35957E-10	6.42196E-08	4.86527E-06	1	1.0762E+10	1.42394E-05	0.93166	
H2O	7.32071E-07	1.99245E-04	1.96657E-02	2	7.6296E+10	2.87317E+00	1.00000	
OH	1.93035E-10	5.25377E-08	4.78803E-06	3	5.9938E+11	2.84734E+00	1.00000	
H	3.74249E-09	1.01858E-06	7.72885E-05	4	2.6434E+13	2.92939E-01	0.93068	
O2	1.22390E-03	3.33105E-01	-2.54053E-02	5	3.1047E+13	2.33083E-02	1.00000	
H2	2.44879E-03	6.66479E-01	-3.22992E-02	6	8.0000E+12	4.91341E-03	1.00000	
H02	3.86994E-07	1.05327E-04	5.95029E-03	7	8.0477E+13	9.58268E-01	1.00000	
H2O2	4.05418E-07	1.10341E-04	9.61734E-03	8	5.3022E+08	3.94675E+00	0.95538	
				9	3.0860E+12	1.98468E-03	0.99955	
				10	1.8000E+12	2.20947E+00	0.99691	
				11	7.8000E+11	9.72995E-03	1.00000	
				12	5.4969E+07	1.20822E+00	1.00000	
				13	2.5930E+12	1.00771E+01	0.99998	
				14	2.3513E+15	1.26972E+01	0.99984	
				15	2.2664E-07	-7.21735E-05	1.00000	
				16	6.7231E+15	2.87269E-06	1.00000	
				17	2.9877E-06	-6.86190E-05	0.99999	
				18	6.4193E-10	-2.43644E-09	0.99999	
DERIVATIVES (FPS UNITS): T 8.43709E+01 RHO 8.54923E-04 V -3.07830E+02								
MIXTURE MOLECULAR WEIGHT	12.01328		TOTAL ENERGY EXCHANGE RATE (BTU-FT**3/LB**2/SEC)	-1.33268E+06	MASS FRACTION SUM	1.00000000		

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 6.099997E-01 S UP TO THIS TIME - 6.099997E-01 S

TABLE D.2.—Continued.
(d) Concluded.

TIME	3.38532E-04	SEC	AREA	2.57048E+00	SQ FT	AXIAL POSITION	5.23319E-01	FT
FLOW PROPERTIES					INTEGRATION INDICATORS			
PRESSURE (LB/FT**2)	1.09185E+04				STEPS FROM LAST PRINT	81		
VELOCITY (FT/SEC)	1.46571E+03				AVERAGE STEP SIZE	0.11319E-01		
DENSITY (LB/FT**3)	4.04266E-02				METHOD ORDER	4		
TEMPERATURE (DEG R)	2117.59							
MASS FLOW RATE (LB/SEC)	1.52297E+02				TOTAL NUMBER OF STEPS	241		
ENTROPY (BTU/LB/DEG R)	3.75331E+00				FUNCT EVALUATIONS	324		
MACH NUMBER	4.29328E-01				JACOBIAN EVALUATIONS	34		
GAMMA	1.34109E+00							
ENTHALPY (BTU/LB)	8.29365E+02							
SP. HEAT (CP) (BTU/LB/DEG R)	6.44879E-01							
HEAT LOSS(QDOT/MDOT) = 5.4439E+00 BTU/(LB-FT)								
CHEMICAL PROPERTIES								
SPECIES	CONCENTRATION (MOLES/FT**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/FT**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-FT**3/LB**2/SEC)	NET RATE/POSI- TIVE DIR RATE	
O	1.50296E-07	4.50428E-05	2.78407E-01	1	2.6351E+10	-4.21688E-01	0.16951	
H2O	5.32254E-05	1.59514E-02	3.25414E+01	2	1.6974E+11	4.09029E+03	0.99887	
OH	2.64514E-07	7.92732E-05	4.90561E-01	3	1.1719E+12	3.76604E+03	0.99818	
H	2.25878E-06	6.76943E-04	4.09676E+00	4	2.9321E+13	2.07131E+03	0.99985	
O2	1.08970E-03	3.26576E-01	-1.55385E+01	5	5.2599E+13	1.53250E+02	1.00000	
H2	2.18564E-03	6.55024E-01	-3.36171E+01	6	8.0000E+12	6.61902E+01	1.00000	
H2O2	3.19142E-06	9.56450E-04	2.02588E-01	7	8.4787E+13	5.99043E+03	1.00000	
	2.30550E-06	6.90946E-04	-1.31927E+00	8	1.7942E+09	-8.56699E+02	0.87476	
				9	3.3088E+12	1.97733E+01	0.99981	
				10	1.8000E+12	1.79476E+02	0.99884	
				11	7.8000E+11	3.98113E+01	1.00000	
				12	5.0566E+08	7.04241E+01	0.99132	
				13	5.4909E+12	1.97505E+04	0.99849	
				14	2.2394E+15	7.88762E+03	0.99997	
				15	3.8180E-05	-5.46610E+01	1.00000	
				16	6.0352E+15	1.07327E+00	1.00000	
				17	3.2231E-04	-1.89787E+01	1.00000	
				18	1.8191E-07	-9.26897E-04	1.00000	
DERIVATIVES (FPS UNITS): T 7.77921E+04 RHO -1.37638E+00 V -3.50268E+02								
MIXTURE MOLECULAR WEIGHT 12.11563 TOTAL ENERGY EXCHANGE RATE -1.765+2E+09 MASS FRACTION SUM 1.00000001								
(BTU-FT**3/LB**2/SEC)								
COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 5.100002E-01 S UP TO THIS TIME - 1.490000E+00 S								
(LSENS) END OF THIS CASE								
SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:								
TOTAL NO. OF STEPS - 241								
TOTAL NO. OF DERIVATIVE EVALUATIONS - 324								
TOTAL NO. OF JACOBIAN EVALUATIONS - 34								
TOTAL CPU TIME - 1.490000 S								
TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 2.640000 S								
(LSENS) READ DATA FOR NEXT CASE								

TABLE D.2.—Continued.

(e) Case 5

TIME-PRESSURE VERSION		LEHIS SENSITIVITY AND GENERAL KINETICS PROGRAM		NASA LEHIS RESEARCH CENTER	
ISENS		CH4 - O2 - H2 MECH. BATCH RXN. WITH OTTO CYCLE HEAT LOSS		CASE 5	
REACTION NUMBER	REACTION	REACTION RATE	VARIABLES	ACTIVATION ENERGY	
1	M	1*CH4	1	2.00000E+17	0.0000
2	1*H	1*CH4	2	1.26000E+14	0.0000
3	1*CH4	1*O2	3	7.94000E+13	0.0000
4	1*O	1*CH4	4	1.90000E+14	0.0000
5	1*OH	1*CH4	5	2.50000E+13	0.0000
6	1*CH3	1*O2	6	2.40000E+13	0.0000
7	1*CH3	1*OH	7	6.30000E+12	0.0000
8	M	1*CH3O	8	5.00000E+13	0.0000
9	M	1*CH3	9	2.40000E+14	0.0000
10	1*H	1*CH3	10	1.52000E+14	0.0000
11	1*O	1*CH3	11	1.15000E+14	0.0000
12	1*OH	1*CH3	12	8.70000E+13	0.0000
13	M	1*CH3	13	1.00000E+17	0.0000
14	1*CH2H5	1*O2	14	2.00000E+12	0.0000
15	1*H	1*CH2H5	15	4.80000E+13	0.0000
16	1*CH3	1*CH2	16	2.00000E+11	0.0000
17	1*H	1*CH2H4	17	1.50000E+14	0.0000
18	M	1*CH2H4	18	2.60000E+17	0.0000
19	1*CH2H4	1*OH	19	4.80000E+12	0.0000
20	1*CH2H4	1*O	20	3.00000E+11	0.0000
21	1*CH2H4	1*O	21	3.00000E+15	0.0000
22	1*CH2H4	1*O	22	3.98000E+12	0.0000
23	M	1*CH2H3	23	6.00000E+12	0.0000
24	1*CH2H3	1*O2	24	3.30000E+13	0.0000
25	1*CH2H3	1*H	25	3.00000E+13	0.0000
26	1*CH2H3	1*O	26	3.00000E+13	0.0000
27	1*CH2H3	1*OH	27	3.00000E+13	0.0000
28	1*CH2H3	1*CH2	28	3.00000E+13	0.0000
29	1*CH2H3	1*CH2H	29	2.00000E+13	0.0000
30	M	1*CH2H2	30	4.20000E+16	0.0000
31	1*CH2H2	1*O	31	1.60000E+14	0.0000
32	1*CH2H2	1*OH	32	4.00000E+14	0.0000
33	1*CH2H2	1*O	33	6.30000E+12	0.0000
34	1*CH2H2	1*OH	34	3.20000E+11	0.0000
35	1*CH2H2	1*O2	35	5.00000E+13	0.0000
36	1*CH2H2	1*OH	36	2.00000E+13	0.0000
37	1*CH2H2	1*O2	37	1.46000E+12	0.0000
38	1*CH2H2	1*O	38	1.20200E+12	0.0000
39	1*CH2H2	1*OH	39	1.00000E+13	0.0000
40	1*CH2H2	1*O	40	3.00000E+13	0.0000
41	1*CH2H2	1*CH2	41	3.00000E+13	0.0000
42	1*CH2H2	1*CH2H	42	1.00000E+13	0.0000
43	1*CH2H2	1*CH2H2	43	1.00000E+13	0.0000
44	1*CH2H2	1*OH	44	2.80000E+13	0.0000
45	1*CH2H2	1*O	45	7.50000E+12	0.0000
46	1*CH2H2	1*H	46	1.15000E+13	0.0000
47	1*CH2H2	1*O	47	7.50000E+13	0.0000
48	1*CH2H2	1*OH	48	5.00000E+13	0.0000
49	1*CH2H2	1*O	49	2.00000E+13	0.0000
50	M	1*CH2H2	50	2.00000E+16	0.0000
51	1*CH2H	1*O	51	5.00000E+13	0.0000
52	1*CH2H	1*O2	52	1.00000E+13	0.0000
53	1*CH2H	1*OH	53	2.00000E+13	0.0000
54	M	1*CH2H	54	5.00000E+16	0.0000
55	1*CH2H	1*OH	55	3.00000E+13	0.0000
56	1*CH2H	1*O	56	2.50000E+13	0.0000
57	1*CH2H	1*O	57	3.50000E+13	0.0000
58	1*CH2H	1*CH2H	58	1.00000E+10	0.5000
59	1*CH2H	1*CH2H	59	3.00000E+11	0.5000
60	1*CH2H	1*CH2H	60	2.00000E+11	0.0000
61	M	1*CH2H	61	1.95000E+16	0.0000
62	1*H	1*CH2H	62	2.70000E+11	0.6700
63	1*O	1*CH2H	63	1.90000E+11	0.6800
64	1*OH	1*CH2H	64	2.70000E+11	0.6700
65	1*CH	1*O2	65	3.70000E+12	0.0000
66	1*CH	1*O	66	1.00000E+11	0.0000
67	1*CH	1*OH	67	2.00000E+11	0.7000
68	1*CH	1*O	68	5.00000E+11	0.5000
69	1*CH	1*OH	69	2.00000E+11	0.7000
70	1*CH	1*O	70	5.00000E+11	0.5000
71	M	1*CH	71	3.20000E+11	0.7000
72	1*H	1*CH	72	5.00000E+12	0.0000
73	1*HCO	1*O2	73	6.00000E+13	0.0000
74	1*HCO	1*O	74	3.00000E+13	0.0000
75	1*HCO	1*OH	75	3.00000E+13	0.0000
76	1*HCO	1*O	76	2.00000E+13	0.0000
77	M	1*HCO	77	2.00000E+14	0.0000
78	1*CO	1*O	78	2.00000E+14	0.0000
79	1*CO	1*O2	79	2.50000E+12	0.0000
80	1*CO	1*OH	80	4.17000E+11	0.0000
81	1*CO	1*O	81	5.75000E+13	0.0000
82	1*O	1*HCO	82	6.80000E+13	0.0000
83	1*H	1*O2	83	1.89000E+14	0.0000
84	1*O	1*H2	84	4.00000E+16	0.0000
85	1*H	1*H2	85	7.80000E+13	0.0000
86	1*O	1*H2	86	5.00000E+13	0.0000
87	1*OH	1*H2	87	8.00000E+12	0.0000
88	1*H	1*H2	88	1.34000E+14	0.0000
89	1*H2	1*H2	89	7.91000E+13	0.0000
90	1*OH	1*H2	90	6.10000E+12	0.0000
91	M	1*H2	91	1.80000E+12	0.0000
92	1*H	1*H2	92	7.80000E+11	0.0000
93	M	1*H2	93	1.44000E+17	0.0000
94	1*H2	1*O	94	4.74000E+13	0.0000
95	1*H	1*O	95	1.66000E+15	0.0000
96	M	1*O	96	1.50000E+15	0.0000
97	1*H	1*O	97	7.10000E+18	-1.0000
98	M	1*O	98	2.20000E+14	0.0000
99	M	1*O	99	1.80000E+18	1.0000
100	1*CH	1*O2	100	1.00000E+11	0.0000
101	1*CH	1*O	101	6.00000E+13	0.0000
102	1*O	1*CH	102	1.00000E+11	0.0000
103	1*OH	1*CH	103	4.00000E+11	0.0000
104	1*CH	1*O	104	1.20000E+13	0.0000
105	1*CH	1*O	105	2.50000E+14	0.0000
106	1*H2	1*CH	106	1.00000E+14	0.0000
107	1*H2	1*O	107	3.00000E+14	0.0000
108	1*H2	1*O	108	1.00000E+14	0.0000
109	1*CH	1*O	109	3.70000E+12	0.0000
110	1*O	1*CH	110	2.00000E+13	0.0000

TABLE D.2.—Continued.
(c) Continued.

111	1*H	+	1*HCO	*	1*H2	+	1*CO	1.00000E+15	0.0000	0.00
112	1*H	+	1*HCO	*	1*HH	+	1*CO	2.00000E+15	0.0000	0.00
113	1*CH	+	1*HCO	*	1*H	+	1*HCO	1.00000E+15	0.0000	9940.00
114	1*CH	+	1*HCO	*	1*H	+	1*HCO	2.00000E+12	0.0000	0.00
115	1*HH	+	1*HCO	*	1*H	+	1*H2O	5.00000E+11	0.5000	2000.00
116	1*H2O	+	1*HCO	*	1*H2O	+	1*OH	2.09000E+12	0.0000	-477.00
117	1*O	+	1*H2O	*	1*H	+	1*O2	1.00000E+13	0.0000	596.00
118	1*H2O	+	1*O	*	1*H2O	+	M	5.62000E+15	0.0000	-1160.00
119	1*H2O	+	1*H	*	1*H	+	1*OH	3.47000E+14	0.0000	1470.00
120	1*H2O	+	1*H	*	1*H	+	1*OH	0.0000	0.0000	50410.00
121	1*H2O	+	1*O	*	1*H	+	1*O2	3.80000E+09	1.0000	41570.00
122	1*O	+	1*H2	*	1*H2O	+	1*H	1.80000E+14	0.0000	76250.00
123	1*H	+	1*H2O	*	2*H2O	+	1*H	4.00000E+12	0.0000	0.00
124	M	+	1*H2O	*	1*H2	+	1*O2	6.92000E+23	2.5000	65000.00
125	1*O	+	1*H2O	*	1*H2	+	1*O2	1.00000E+14	0.0000	78020.00
126	1*O	+	1*H2O	*	2*H2O	+	1*O2	6.92000E+13	0.0000	26630.00
127	1*H2O	+	1*H	*	1*H2	+	1*OH	7.57000E+13	0.0000	15100.00
128	1*H2O	+	1*H2	*	1*H2O2	+	1*H	2.40000E+13	0.0000	29000.00
129	1*OH	+	1*H2O	*	1*H2O3	+	M	3.00000E+15	0.0000	-3800.00
130	1*OH	+	1*H2O	*	1*H2O2	+	M	5.60000E+15	0.0000	-1700.00
131	1*HHO	+	1*H	*	1*H2	+	1*H2O	5.00000E+12	0.0000	0.00
132	1*H	+	1*H2O	*	1*HHO	+	M	5.40000E+05	0.0000	640.00
133	1*HHO	+	1*OH	*	1*H2O	+	1*H2O	3.60000E+13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

MCH2	, 93) =	2.50000	MCO2	, 93) =	0.78000	MCH2O	, 93) =	6.00000	MCH2O2	, 93) =	6.60000
MCO2	, 95) =	1.30000	MCH2	, 95) =	1.30000	MCH2O	, 95) =	21.30000	MCH2O2	, 95) =	7.00000
MCH2	, 96) =	4.00000	MCO2	, 96) =	1.50000	MCH2O	, 96) =	20.00000	MCH2	, 96) =	1.50000
MCO2O2	, 96) =	4.00000	MCH2	, 98) =	4.10000	MCO2	, 98) =	2.00000	MCH2O	, 98) =	15.00000
MCH2	, 98) =	2.00000	MCO2	, 129) =	0.70000	MCH2	, 129) =	1.40000			

TRANSPORT PROPERTY COEFFICIENTS

H2	0.687200E+00	-0.617320E+00	-0.111490E+05	0.577240E+00	VI5C
H2	0.116129E+01	0.469043E+03	0.551496E+05	-0.149041E+01	COND
CH4	0.600440E+00	-0.817476E+02	0.165196E+04	0.154710E+01	VI5C
CH4	0.853201E+00	-0.288931E+03	0.193692E+05	0.255748E+00	COND
C2H2	0.579032E+00	0.152664E+03	0.628889E+04	0.177748E+01	VI5C
C2H2	0.666734E+00	-0.330498E+03	0.165066E+05	0.118596E+01	COND
C2H4	0.578808E+00	-0.148526E+03	0.598107E+04	0.175623E+01	VI5C
C2H4	0.674458E+00	-0.506382E+03	0.309615E+05	0.150244E+01	COND
HO	0.646504E+00	0.388567E+01	-0.858737E+04	0.165204E+01	VI5C
HO	0.614175E+00	0.260519E+03	0.360173E+05	0.110633E+01	COND
H2	0.635933E+00	-0.119153E+02	-0.471490E+04	0.166605E+01	VI5C
H2	0.686593E+00	-0.161885E+03	0.236277E+05	0.482688E+00	COND
O	0.763927E+00	0.569723E+02	-0.345462E+04	0.822320E+00	VI5C
O	0.776744E+00	0.803466E+02	-0.349619E+04	-0.481407E+01	COND
H	0.860209E+00	0.498177E+02	-0.542523E+04	-0.102876E+01	VI5C
H	0.869708E+00	0.670316E+02	-0.828927E+04	0.891354E+00	COND
H2O	0.756180E+00	-0.301892E+03	0.187539E+05	0.987951E+00	VI5C
H2O	0.123241E+01	0.163667E+03	0.141541E+05	-0.291285E+01	COND
HO2	0.603384E+00	0.988315E+02	-0.969625E+03	0.200464E+01	VI5C
HO2	0.504502E+00	-0.475725E+03	0.415525E+05	0.201241E+01	COND
OH	0.597497E+00	-0.365001E+03	0.351550E+05	0.217217E+01	VI5C
OH	0.812287E+00	0.264950E+03	0.343595E+05	0.105187E+00	COND
CO	0.779825E+00	0.193974E+03	-0.317845E+05	0.456375E+00	VI5C
CO	0.800546E+00	0.237400E+02	0.804541E+04	-0.468414E+00	COND
CO2	0.440370E+00	-0.288400E+03	0.193120E+05	0.324659E+01	VI5C
CO2	0.603518E+00	0.438483E+03	0.322949E+05	0.134023E+01	COND
O2	0.659260E+00	0.941422E+00	-0.711780E+04	0.164435E+01	VI5C
O2	0.478050E+00	-0.452958E+03	0.579015E+05	0.228192E+01	COND

TABLE D.2.—Continued.
(c) Continued.

** INITIAL CONDITIONS **									
TIME	0.00000E+00	SEC	AREA	0.00000E+00	SQ CM	AXIAL POSITION	0.00000E+00	CM	
FLOW PROPERTIES					INTEGRATION INDICATORS				
PRESSURE	2.00000				STEPS FROM LAST PRINT	0			
(ATM)					AVERAGE STEP SIZE	0.00000E+00			
VELOCITY	0.00				METHOD ORDER	0			
(CM/SEC)									
DENSITY	4.18827E-04				TOTAL NUMBER OF STEPS	0			
(G/CM**3)					FNCT EVALUATIONS	0			
TEMPERATURE	1550.00				JACOBIAN EVALUATIONS	0			
(DEG K)									
MASS FLOW RATE	0.00000E+00								
(G/SEC)									
ENTROPY	2.2819								
(CAL/G-DEG K)									
MACH NUMBER	0.0000								
GAMMA	1.2285								
ENTHALPY	3.15126E+02								
(CAL/G)									
SP. HEAT (CP)	4.01086E-01								
(CAL/G-DEG K)									
HEAT LOSS(QDOT/TOTMAS) = 3.3606E+02 CAL/(G-SEC)									
CHEMICAL PROPERTIES									
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE		
CH4	2.71255E-06	1.72500E-01	-1.07574E-05	1	7.8170E+04	1.9081E+01	0.00000		
CH3	0.00000E+00	0.00000E+00	1.07574E-05	2	2.6455E+12	0.00000E+00	0.00000		
H	0.00000E+00	0.00000E+00	3.45795E-06	3	1.0089E+06	4.2316E+01	1.00000		
H2	0.00000E+00	0.00000E+00	9.89090E-07	4	4.2290E+12	0.00000E+00	0.00000		
O2	2.71255E-06	1.72500E-01	2.40725E-02	5	4.9151E+12	0.00000E+00	0.00000		
H2O	0.00000E+00	0.00000E+00	7.42305E-06	6	2.1694E+09	0.00000E+00	0.00000		
O	0.00000E+00	0.00000E+00	2.40649E-02	7	6.3000E+12	0.00000E+00	0.00000		
OH	0.00000E+00	0.00000E+00	0.00000E+00	8	5.4698E+10	0.00000E+00	0.00000		
H2O	0.00000E+00	0.00000E+00	0.00000E+00	9	1.2708E+13	0.00000E+00	0.00000		
CH3O	0.00000E+00	0.00000E+00	0.00000E+00	10	5.6608E+12	0.00000E+00	0.00000		
CH2O	0.00000E+00	0.00000E+00	8.76480E-04	11	8.8155E+12	0.00000E+00	0.00000		
CH3H	0.00000E+00	0.00000E+00	0.00000E+00	12	2.7746E+13	0.00000E+00	0.00000		
CH2H	0.00000E+00	0.00000E+00	0.00000E+00	13	4.2560E+12	0.00000E+00	0.00000		
CH2H	0.00000E+00	0.00000E+00	0.00000E+00	14	3.9449E+11	0.00000E+00	0.00000		
CH2	1.57249E-10	1.00000E-05	8.78705E-04	15	4.8000E+13	0.00000E+00	0.00000		
CH3	0.00000E+00	0.00000E+00	1.23656E-07	16	2.0000E+13	0.00000E+00	0.00000		
CH2H	0.00000E+00	0.00000E+00	9.89090E-07	17	5.4688E+12	0.00000E+00	0.00000		
HCH	0.00000E+00	0.00000E+00	1.27964E-02	18	1.7127E+06	0.00000E+00	0.00000		
CH2H2O	0.00000E+00	0.00000E+00	0.00000E+00	19	3.2197E+12	0.00000E+00	0.00000		
CH	0.00000E+00	0.00000E+00	0.00000E+00	20	1.4644E+12	0.00000E+00	0.00000		
CO	0.00000E+00	0.00000E+00	0.00000E+00	21	2.2866E+12	0.00000E+00	0.00000		
CH2H	0.00000E+00	0.00000E+00	0.00000E+00	22	4.9311E+12	0.00000E+00	0.00000		
CH	4.71747E-10	3.00000E-05	-1.27974E-02	23	9.2284E+10	0.00000E+00	0.00000		
CO2	0.00000E+00	0.00000E+00	0.00000E+00	24	4.3165E+12	0.00000E+00	0.00000		
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	25	6.0000E+12	0.00000E+00	0.00000		
H2	1.02786E-05	6.54920E-01	-1.01739E-04	26	3.3000E+13	0.00000E+00	0.00000		
HCH	0.00000E+00	0.00000E+00	1.01739E-04	27	5.0000E+12	0.00000E+00	0.00000		
H	1.57249E-10	1.00000E-05	-5.25625E-04	28	3.0000E+13	0.00000E+00	0.00000		
CH	1.57249E-10	1.00000E-05	-9.86541E-03	29	3.0000E+13	0.00000E+00	0.00000		
HNCO	0.00000E+00	0.00000E+00	0.00000E+00	30	3.4377E+01	0.00000E+00	0.00000		
HCO	0.00000E+00	0.00000E+00	9.86541E-03	31	6.4511E+12	0.00000E+00	0.00000		
HN2	0.00000E+00	0.00000E+00	0.00000E+00	32	1.2560E+13	0.00000E+00	0.00000		
HO	0.00000E+00	0.00000E+00	5.26643E-04	33	6.4914E+11	0.00000E+00	0.00000		
NH	0.00000E+00	0.00000E+00	0.00000E+00	34	2.9988E+11	0.00000E+00	0.00000		
H2O	0.00000E+00	0.00000E+00	0.00000E+00	35	3.0723E+13	0.00000E+00	0.00000		
H2O	0.00000E+00	0.00000E+00	6.36740E-13	36	2.0000E+13	0.00000E+00	0.00000		
HNH2	0.00000E+00	0.00000E+00	0.00000E+00	37	6.4842E+11	0.00000E+00	0.00000		
HNH3	0.00000E+00	0.00000E+00	0.00000E+00	38	1.2020E+12	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	39	1.0000E+13	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	40	5.0000E+13	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	41	3.0000E+13	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	42	5.2246E+12	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	43	1.0000E+13	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	44	2.8000E+13	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	45	2.8318E+12	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	46	3.7131E+12	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	47	5.5855E+12	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	48	3.237E+12	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	49	2.0000E+13	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	50	6.9349E+07	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	51	5.0000E+13	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	52	9.7506E+11	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	53	2.0000E+13	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	54	1.8566E+05	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	55	2.0320E+13	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	56	6.8446E+12	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	57	1.1235E+13	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	58	5.6126E+10	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	59	1.1811E+13	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	60	2.0000E+13	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	61	2.3684E+03	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	62	8.8143E+09	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	63	6.6755E+09	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	64	8.8143E+09	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	65	3.7000E+12	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	66	1.0000E+13	7.2948E+04	1.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	67	2.0548E+12	4.9965E+03	1.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	68	7.8789E+09	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	69	2.8989E+12	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	70	1.0905E+13	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	71	5.0000E+12	7.06819E-01	1.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	72	4.0000E+13	5.4255E+00	1.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	73	5.0000E+13	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	74	5.0000E+13	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	75	5.0000E+13	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	76	2.0000E+13	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	77	1.8494E+12	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	78	6.3403E+14	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	79	4.7162E+05	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	80	5.0140E+11	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	81	3.3616E+10	0.00000E+00	0.00000		
HNH	0.00000E+00	0.00000E+00	0.00000E+00	82	1.7500E+11	0.00000E+00	0.00000		

TABLE D.2.—Continued.
(c) Continued.

83	9.2051E+11	0.00000E+00	0.00000
84	4.8361E+12	0.00000E+00	0.00000
85	3.6501E+13	0.00000E+00	0.00000
86	3.1151E+13	0.00000E+00	0.00000
87	8.0000E+12	0.00000E+00	0.00000
88	9.4671E+13	0.00000E+00	0.00000
89	2.3615E+10	0.00000E+00	0.00000
90	3.8344E+12	0.00000E+00	0.00000
91	1.8000E+12	0.00000E+00	0.00000
92	7.8000E+11	0.00000E+00	0.00000
93	5.5151E+10	0.00000E+00	0.00000
94	6.5458E+12	0.00000E+00	0.00000
95	2.0200E+15	0.00000E+00	0.00000
96	1.9463E+00	0.00000E+00	0.00000
97	4.5806E+15	0.00000E+00	0.00000
98	6.4058E+00	0.00000E+00	0.00000
99	2.6554E-02	6.4570E-06	0.00000
100	2.0941E+08	5.7998E+00	1.00000
101	1.0736E+13	0.00000E+00	0.00000
102	8.5636E+10	0.00000E+00	0.00000
103	1.6111E+11	0.00000E+00	0.00000
104	1.2000E+13	0.00000E+00	0.00000
105	3.5648E+13	0.00000E+00	0.00000
106	5.3821E+12	0.00000E+00	0.00000
107	6.3311E+12	0.00000E+00	0.00000
108	2.3124E+13	5.6240E+04	1.00000
109	3.7000E+12	0.00000E+00	0.00000
110	2.0000E+13	0.00000E+00	0.00000
111	1.0000E+13	0.00000E+00	0.00000
112	2.0000E+13	0.00000E+00	0.00000
113	6.3471E+11	0.00000E+00	0.00000
114	2.0000E+12	0.00000E+00	0.00000
115	1.0281E+13	0.00000E+00	0.00000
116	2.4401E+12	0.00000E+00	0.00000
117	8.2407E+12	0.00000E+00	0.00000
118	8.1902E+15	0.00000E+00	0.00000
119	2.1531E+14	0.00000E+00	0.00000
120	2.0519E+07	0.00000E+00	0.00000
121	8.6481E+06	-3.0022E+03	1.00000
122	3.1918E+05	0.00000E+00	0.00000
123	4.0000E+12	0.00000E+00	0.00000
124	5.0036E+06	0.00000E+00	0.00000
125	1.1199E+10	-3.6298E-06	1.00000
126	1.2170E+10	0.00000E+00	0.00000
127	5.6387E+11	0.00000E+00	0.00000
128	1.9551E+09	0.00000E+00	0.00000
129	1.0301E+16	0.00000E+00	0.00000
130	9.7251E+15	0.00000E+00	0.00000
131	5.0000E+12	0.00000E+00	0.00000
132	6.5611E+15	0.00000E+00	0.00000
133	3.6000E+13	0.00000E+00	0.00000
DERIVATIVES (CGS UNITS): T	6.22257E+06	RHO	-1.53490E+00
MIXTURE MOLECULAR WEIGHT	26.63461	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	-6.00627E+09
		MASS FRACTION SUM	1.00000000
CPU TIME FOR INITIALIZATION OF ISENS = 2.36000 S			
REYNOLDS NUMBER = 3.8301E+03	PRANDTL NUMBER = 0.722	HEAT TRANSFER COEFF = 5.43804E-04	
REYNOLDS NUMBER = 3.8295E+03	PRANDTL NUMBER = 0.722	HEAT TRANSFER COEFF = 5.43781E-04	
REYNOLDS NUMBER = 3.8290E+03	PRANDTL NUMBER = 0.722	HEAT TRANSFER COEFF = 5.43757E-04	
REYNOLDS NUMBER = 3.8289E+03	PRANDTL NUMBER = 0.722	HEAT TRANSFER COEFF = 5.43748E-04	
REYNOLDS NUMBER = 3.8290E+03	PRANDTL NUMBER = 0.722	HEAT TRANSFER COEFF = 5.43774E-04	
REYNOLDS NUMBER = 3.8296E+03	PRANDTL NUMBER = 0.722	HEAT TRANSFER COEFF = 5.43875E-04	
REYNOLDS NUMBER = 3.8302E+03	PRANDTL NUMBER = 0.722	HEAT TRANSFER COEFF = 5.43971E-04	
REYNOLDS NUMBER = 3.8315E+03	PRANDTL NUMBER = 0.722	HEAT TRANSFER COEFF = 5.44174E-04	
REYNOLDS NUMBER = 3.8435E+03	PRANDTL NUMBER = 0.722	HEAT TRANSFER COEFF = 5.46018E-04	
REYNOLDS NUMBER = 3.9190E+03	PRANDTL NUMBER = 0.722	HEAT TRANSFER COEFF = 5.57572E-04	
TIME 2.50000E-04 SEC	AREA 0.00000E+00 SQ CM	AXIAL POSITION 0.00000E+00 CM	
FLOW PROPERTIES		INTEGRATION INDICATORS	
PRESSURE (ATM)	2.17500	STEPS FROM LAST PRINT	177
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.14198E-05
DENSITY (G/CM**3)	4.46455E-04	METHOD ORDER	4
TEMPERATURE (DEG K)	1581.40		
MASS FLOW RATE (G/SEC)	0.00000E+00	TOTAL NUMBER OF STEPS	177
ENTROPY (CAL/G/DEG K)	2.2856	FUNCTION EVALUATIONS	211
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	27
GAMMA	1.2273		
ENTHALPY (CAL/G)	3.24834E+02		
SP. HEAT (CP) (CAL/G/DEG K)	4.02837E-01		
HEAT LOSS(QBDI/101MAS) =	3.5278E+02	CAL/(G-SEC)	
CHEMICAL PROPERTIES			
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)
CH4	2.85311E-06	1.70224E-01	-2.52423E-04
CH3	4.30681E-09	2.56956E-04	1.60071E-05
H	4.55929E-12	2.72019E-07	2.18857E-08
H2	4.84210E-09	2.88893E-04	3.45887E-05
			REACTION NUMBER
			1
			2
			3
			4
			RATE CONST CGS UNITS
			1.3786E+05
			2.8562E+12
			1.4475E+06
			4.5609E+12
			NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)
			3.24282E+01
			1.75561E+02
			4.89553E+01
			2.23457E+02
			NET RATE/POSTIVE DIR RATE
			0.98045
			0.93111
			0.82341
			0.99983

TABLE D.2.—Continued.
(e) Continued.

DZ	2.86958E-06	1.71195E-01	-1.50269E-04	5	5.0764E+12	8.09378E+02	0.99982
HOZ	1.15893E-09	6.91451E-05	1.34298E-06	6	2.6100E+09	1.61769E+02	0.99969
U	3.42356E-12	2.04247E-07	1.47194E-08	7	6.5009E+12	-1.19526E+01	0.88671
OH	1.11965E-11	6.68014E-07	5.29820E-08	8	6.2629E+10	1.71413E+02	1.00000
H2O	2.34795E-08	1.40084E-03	1.68188E-04	9	1.2606E+13	2.66781E+02	0.22741
CH3O	3.25682E-11	1.94191E-06	1.45999E-07	10	6.0261E+12	1.12042E+00	0.99999
CH2O	1.67694E-08	1.00051E-03	1.19800E-04	11	9.2942E+12	1.29753E+00	1.00000
C2H6	8.12846E-09	4.84966E-04	5.01102E-05	12	2.8383E+13	1.51884E+01	0.99999
C2H5	3.50933E-14	2.09376E-09	2.90382E-10	13	5.1974E+12	1.29596E+01	1.00000
C2H4	2.55090E-10	1.52194E-05	3.40857E-06	14	4.0741E+11	1.87688E-01	0.99999
CH2	8.88046E-16	5.29832E-11	1.40189E-11	15	4.8000E+13	3.72064E-05	0.96563
C2H3	1.12477E-15	6.71066E-11	2.06752E-11	16	2.0000E+13	3.83611E-04	0.99960
C2H2	8.61795E-13	5.14170E-08	1.42724E-08	17	5.8405E+12	3.40765E-02	0.99992
HCO	7.80929E-14	4.65925E-09	8.29057E-10	18	2.8538E+06	6.12585E-02	1.00000
C2H2O	7.68740E-15	4.58651E-10	1.16384E-10	19	3.2453E+12	4.65023E-02	0.99999
C2H	7.35539E-20	4.38842E-15	2.24083E-15	20	1.4735E+12	-1.89858E+00	0.78900
CO	1.14765E-09	6.84719E-05	9.33697E-06	21	2.3033E+12	1.00911E-02	1.00000
C2H	2.44409E-17	1.45821E-12	5.21570E-13	22	5.0926E+12	2.23108E-02	0.99996
CH	2.66284E-21	1.58872E-16	6.36807E-17	23	1.1343E+11	1.06944E-02	0.99683
CO2	1.97891E-11	1.18067E-06	7.17669E-08	24	4.3096E+12	6.97796E-02	1.00000
H2O2	2.13958E-12	1.27653E-07	2.90198E-09	25	6.0000E+12	1.52647E-07	1.00000
H2	1.09779E-05	6.54971E-01	-1.65843E-11	26	3.3000E+13	6.37491E-07	1.00000
HCN	4.80586E-14	2.86731E-09	5.57553E-11	27	5.0000E+12	3.15643E-07	0.99916
N	3.05455E-17	1.81036E-12	1.55584E-13	28	3.0000E+13	-8.94469E-09	0.98367
CH	2.13920E-16	1.27630E-11	-8.30707E-12	29	3.0000E+13	1.01771E-04	1.00000
HNC	1.53601E-10	9.15229E-06	3.18111E-07	30	6.8758E+12	-5.78078E-15	0.25291
HCO	1.17065E-11	6.98429E-07	-3.24701E-07	31	6.8758E+12	4.95006E-09	0.99737
H2	3.78526E-13	2.25839E-08	4.67378E-09	32	1.3454E+13	1.99137E-04	1.00000
HU	1.08959E-10	6.50081E-06	-1.66719E-07	33	6.7911E+11	5.28545E-05	0.99936
NH	9.91090E-13	5.91311E-08	1.67455E-07	34	3.0027E+11	1.45351E-05	0.99994
H2O	5.94447E-11	3.54663E-06	1.67455E-07	35	3.1022E+13	3.28480E-05	1.00000
N2O	2.60224E-15	1.55256E-10	1.64957E-11	36	2.0000E+13	8.24984E-13	0.99835
HNO2	1.92629E-16	1.14928E-11	1.49045E-12	37	6.5895E+11	2.51849E-04	1.00000
HNO3	5.58837E-18	2.14092E-13	1.95458E-14	38	1.2020E+12	5.04569E-10	1.00000
HNO	4.36919E-16	2.60677E-11	8.85195E-13	39	1.0000E+13	1.37213E-08	0.99963
				40	5.0000E+13	2.34844E-08	0.84014
				41	3.0000E+13	3.26669E-12	0.99997
				42	5.2918E+12	1.21985E-11	0.95489
				43	1.0000E+13	2.99696E-14	1.00000
				44	2.8000E+13	-4.95879E-04	0.97620
				45	2.8871E+12	1.22344E-06	0.98133
				46	3.7960E+12	-1.43264E-04	0.99536
				47	5.8812E+12	7.77150E-07	0.75149
				48	3.9208E+12	5.17343E-07	0.99938
				49	2.0000E+13	7.64062E-06	1.00000
				50	1.0210E+08	6.52580E-05	0.98871
				51	5.0000E+13	6.51646E-11	1.00000
				52	1.0212E+12	4.78484E+02	1.00000
				53	2.0000E+13	1.48901E-02	1.00000
				54	3.1973E+05	4.50866E-01	1.00000
				55	2.0478E+13	1.92897E+01	1.00000
				56	7.0230E+12	2.69589E+00	1.00000
				57	1.1491E+13	5.30966E+00	1.00000
				58	5.8928E+10	2.13510E+01	0.99995
				59	1.1930E+13	2.01204E-02	0.99950
				60	2.0000E+13	5.00828E+02	1.00000
				61	4.2750E+03	1.56213E-03	0.99995
				62	1.0544E+10	1.03850E-03	0.99982
				63	7.9867E+09	5.90774E-04	1.00000
				64	1.0544E+10	2.55073E-03	0.99999
				65	3.7000E+12	7.88303E-13	0.80589
				66	1.0000E+13	3.83334E-07	1.00000
				67	2.1708E+12	2.77517E-07	1.00000
				68	9.4364E+09	1.43926E-10	1.00000
				69	3.0617E+12	1.51722E-07	0.99994
				70	1.1419E+13	2.31744E-07	0.99918
				71	5.0000E+12	1.97793E-11	0.99983
				72	4.0000E+13	1.58261E-10	1.00000
				73	3.0000E+13	3.37231E-01	0.99991
				74	3.0000E+13	4.02375E-05	1.00000
				75	5.0000E+13	1.31601E-04	1.00000
				76	2.0000E+13	3.57247E-05	0.99997
				77	2.0447E+12	1.34269E+01	0.99999
				78	6.5102E+14	2.15077E-04	0.99999
				79	6.4149E+05	1.05983E-02	1.00000
				80	3.0334E+11	1.95405E-02	0.99922
				81	3.8971E+10	2.60052E-01	1.00000
				82	1.9700E+11	7.67928E-02	0.96665
				83	1.0233E+12	6.71583E+01	0.99996
				84	5.2845E+12	4.38314E-01	0.99749
				85	3.7010E+13	5.98356E-01	0.99987
				86	3.6372E+13	7.23273E-01	0.99702
				87	8.0000E+12	5.05542E-01	0.97069
				88	9.5330E+13	2.52715E+00	1.00000
				89	2.7745E+10	7.79485E-01	0.99790
				90	3.8699E+12	-1.62040E-02	0.97210
				91	1.8000E+12	1.21195E+01	0.99918
				92	7.8000E+11	3.81738E-05	1.00000
				93	7.3942E+10	1.29004E+01	1.00000
				94	6.8083E+12	1.71270E+00	0.92488
				95	2.0070E+15	-2.26033E+01	0.88915
				96	3.8337E+00	-3.03366E-05	0.73360
				97	4.4897E+15	5.84064E-06	0.99118
				98	1.1892E+01	6.40088E-06	0.71586
				99	5.5705E-02	1.33869E-05	0.99600
100	2.3670E+08				3.46777E-11		0.99894
101	1.1109E+13				5.76083E-05		0.99784
102	9.6806E+10				-1.29648E-08		0.33960
103	1.6410E+11				-2.22104E-04		1.00000
104	1.2000E+13				4.40890E-08		1.00000
105	3.7046E+13				-3.06725E-04		0.99855
106	5.7043E+12				1.61964E+00		0.99843
107	6.6881E+12				2.34484E-02		0.99918
108	2.3278E+13				6.99404E-02		0.97565
109	3.7000E+12				-6.96497E-02		1.00000
110	2.9000E+13				4.02112E-03		1.00000
111	1.0000E+13				1.78208E-08		1.00000
112	2.0000E+13				5.35532E-03		0.99999
113	6.7673E+11				9.84929E-15		0.99986
114	2.0000E+12				2.90564E-12		0.99800
115	1.0522E+13				5.85767E-06		0.99998
116	2.4326E+12				1.53201E+00		0.99409
117	8.7724E+12				7.06890E-03		0.85660
118	8.1292E+15				-3.84982E-01		0.99934
119	2.1736E+14				2.95548E-01		0.99999
120	2.8390E+07				2.99437E-07		0.04174
121	1.1521E+07				-5.85641E-04		0.99996
122	5.2184E+03				4.61519E-07		0.66907
123	4.0000E+12				3.61974E-08		0.99999
124	7.2362E+06				-7.54880E-05		0.97945

TABLE D.2.—Continued.
(e) Continued.

				125	1.34171110	-7.29295E-06	0.99992
				126	1.44491110	4.92704E-10	0.76218
				127	6.21481111	2.11138E-08	0.57076
				128	2.3573109	3.40413E-03	0.99999
				129	1.0053E+16	9.80617E-08	0.00018
				130	9.6190E+15	-5.39665E-03	0.77489
				131	5.0000E+12	-1.29143E-07	0.72101
				132	6.5360E+15	4.94768E-06	0.01812
				133	3.6000E+13	6.45631E-07	0.73072
DERIVATIVES (CGS UNITS): T							
		1.44692E+05	RHO	1.02827E-01			
MIXTURE MOLECULAR WEIGHT							
	26.63670	TOTAL ENERGY EXCHANGE RATE		-4.613821E+07		MASS FRACTION SUM	1.00000000
		(CAL-CM**3/G**2/SEC)					
COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 1.356000E+01 S UP TO THIS TIME - 1.356000E+01 S							
TIME	3.80000E-04 SEC	AREA	0.00000E+00 SQ CM	AXIAL POSITION	0.00000E+00 CM		
FLOW PROPERTIES				INTEGRATION INDICATORS			
PRESSURE (ATM)	2.26600	STEPS FROM LAST PRINT		4			
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE		0.95497E-05			
DENSITY (G/CM**3)	4.58842E-04	METHOD ORDER		4			
TEMPERATURE (DEG K)	1403.00	TOTAL NUMBER OF STEPS		190			
MASS FLOW RATE (G/SEC)	0.00000E+00	FUNCT EVALUATIONS		232			
ENTROPY (CAL/G/DEG K)	2.2899	JACOBIAN EVALUATIONS		28			
MACH NUMBER	0.0000						
GAMMA	1.2265						
ENTHALPY (CAL/G)	3.29654E+02						
SP. HEAT (CP) (CAL/G/DEG K)	4.03946E-01						
HEAT LOSS(QDOT/TOTMAS) = 3.6518E+02 CAL/(G-SEC)							
CHEMICAL PROPERTIES							
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST (G-UNITS)	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
CH4	2.88586E-06	1.67520E-01	-4.82629E-04	1	2.0103E+05	4.54497E+01	0.95745
CH3	7.16096E-09	4.15684E-04	2.72195E-05	2	3.0057E+12	3.37791E-02	0.86841
H	9.44129E-12	5.48054E-07	5.68900E-08	3	1.8402E+06	5.29514E+01	0.71882
H2	1.16588E-08	6.76774E-04	7.26359E-05	4	4.7959E+12	4.14859E+02	0.99971
O2	2.92036E-06	1.69523E-01	-3.06580E-04	5	5.1866E+12	1.52173E+03	0.98872
HO2	1.43687E-09	8.34084E-05	2.52978E-06	6	2.9514E+09	2.92999E+02	0.99944
O	6.31264E-12	3.66440E-07	3.04531E-08	7	6.3000E+12	-4.18674E+01	0.90025
OH	2.16486E-11	1.25667E-06	1.14853E-07	8	6.8528E+10	3.40390E+02	1.00000
H2O	5.64924E-08	3.27930E-03	3.50123E-04	9	1.2538E+13	4.63634E+02	0.15182
CH3O	6.07057E-11	3.52388E-06	2.95168E-07	10	6.2819E+12	4.79305E+00	0.99998
CH2O	3.87673E-08	2.25038E-03	2.17101E-04	11	9.6122E+12	4.90377E+00	1.00000
C2H6	1.70146E-08	9.87676E-04	8.49566E-05	12	2.8814E+13	5.04120E+01	1.00000
C2H5	1.25432E-13	7.28117E-09	1.18897E-09	13	5.9362E+12	5.94914E+01	0.97645
C2H4	1.24779E-09	7.24325E-05	1.38887E-05	14	4.1623E+11	6.11498E-01	0.84438
CH2	6.72284E-15	3.90251E-10	1.05560E-10	15	4.8000E+13	2.50331E-04	0.92717
C2H3	1.07956E-14	6.26667E-10	1.84743E-10	16	2.0000E+13	4.57137E-03	0.99558
C2H2	7.07630E-12	4.10769E-07	1.09221E-07	17	6.1016E+12	3.41357E-01	0.99982
HCO	3.19879E-13	1.85685E-08	3.40938E-09	18	4.0118E+06	4.09607E-01	1.00000
C2H2O	6.54205E-14	3.79757E-09	1.07426E-09	19	3.2625E+12	4.18585E-01	0.99998
C2H	1.17378E-18	6.81363E-14	2.84774E-14	20	1.4796E+12	-7.31149E+00	0.97469
CO	3.97024E-09	2.30467E-04	3.98261E-05	21	2.3145E+12	8.65920E-02	1.00000
C2HO	3.78074E-16	2.19466E-11	7.84855E-12	22	5.2029E+12	1.94643E-01	0.99992
CH	4.11860E-20	2.39079E-15	9.14900E-16	23	1.3011E+11	1.14396E-01	0.99538
CO2	3.89344E-11	2.26008E-06	2.81059E-07	24	4.3049E+12	6.44649E-01	1.00000
H2O2	2.79110E-12	1.62020E-07	6.54427E-09	25	6.0000E+12	2.86320E-06	0.98571
H2	1.12825E-05	6.54932E-01	-3.44228E-11	26	3.3000E+13	1.06818E-05	1.00000
HCH	5.93685E-14	3.44625E-09	1.07598E-10	27	5.0000E+12	5.54353E-06	0.99878
H	5.78177E-17	3.35624E-12	2.79034E-13	28	3.0000E+13	-1.44198E-07	0.93508
CN	2.89114E-18	1.67826E-13	1.69649E-12	29	3.0000E+13	3.40441E-13	0.18854
HNCO	1.68587E-10	9.78622E-06	-9.01295E-09	30	1.0840E+02	6.24103E-08	0.99431
HCO	4.82385E-14	2.80018E-09	-2.09922E-09	31	7.1735E+12	1.52204E-03	1.00000
HN2	1.36719E-12	7.93636E-08	1.09877E-08	32	1.4083E+13	2.98803E-03	1.00000
HO	9.79850E-11	5.68789E-06	-4.13025E-08	33	6.9980E+11	5.08423E-04	0.99849
HH	1.03340E-12	5.99872E-08	-2.29972E-10	34	3.0053E+11	2.18656E-04	0.99993
HO2	7.51410E-11	4.36183E-06	4.15427E-08	35	3.1222E+13	5.08346E-04	1.00000
H2O	5.84091E-15	3.39056E-10	3.40858E-11	36	2.0000E+13	2.40882E-09	0.99789
HHO2	4.76105E-16	2.76372E-11	2.74619E-12	37	6.6605E+11	3.49296E-03	1.00000
HHO3	7.23725E-18	4.20112E-13	1.10586E-14	38	1.2020E+12	1.36259E-08	1.00000
HHO	6.55848E-16	3.79550E-11	2.52944E-12	39	1.0000E+13	3.88617E-07	0.99964
				40	5.0000E+13	7.23644E-07	0.85366
				41	3.0000E+13	3.62176E-10	0.99999
				42	5.3373E+12	-4.43154E-10	0.87306
				43	1.0000E+13	6.78932E-12	1.00000
				44	2.8000E+13	-4.71936E-03	0.96162
				45	2.9245E+12	1.87676E-05	0.95595
				46	3.8522E+12	-9.16916E-06	0.98782
				47	6.0863E+12	8.27268E-04	0.46331
				48	4.0575E+12	7.94950E-06	0.99880
				49	2.0000E+13	3.92308E-05	1.00000
				50	1.5505E+08	6.88898E-04	0.97461
				51	5.0000E+13	1.75971E-09	1.00000
				52	1.0531E+12	8.86733E+02	1.00000
				53	2.0000E+13	5.44458E-02	1.00000
				54	4.5244E+05	1.45520E+00	1.00000
				55	2.0583E+13	8.20509E+01	1.00000
				56	7.1441E+12	1.26199E+01	0.99999
				57	1.1663E+13	1.15592E+01	1.00000
				58	6.0875E+10	8.02643E-01	0.99994
				59	1.2011E+13	1.30633E-01	0.99962
				60	2.0000E+13	9.77447E+02	1.00000

TABLE D.2.—Continued.

(e) Concluded.

61	6.3304E+03	3.70820E-03	0.99969
62	1.1879E+10	3.81096E-03	0.99994
63	8.9994E+09	1.93227E-03	1.00000
64	1.1879E+10	8.74606E-03	0.99992
65	3.7000E+12	2.48042E-11	0.88017
66	1.0000E+13	5.71294E-06	1.00000
67	2.2518E+12	2.09983E-01	1.00000
68	1.0640E+10	2.14681E-09	1.00000
69	3.1408E+12	2.17081E-06	0.99983
70	1.1776E+13	3.54322E-06	0.99802
71	5.0000E+12	1.07329E-09	0.99992
72	4.0000E+13	8.58696E-09	1.00000
73	3.0000E+13	1.33098E+02	0.99989
74	3.0000E+13	2.87754E-04	1.00000
75	3.0000E+13	9.86753E-04	1.00000
76	2.0000E+13	2.86879E-04	0.99995
77	2.1858E+12	5.72099E+01	0.99998
78	6.6256E+14	1.35873E-03	1.00000
79	7.8698E+05	4.33403E-02	1.00000
80	3.0465E+11	1.74306E-01	0.99948
81	4.2096E+10	1.16503E+00	1.00000
82	2.1314E+11	3.51582E-01	0.97366
83	1.0978E+12	1.43758E+02	0.99994
84	5.6053E+12	1.95506E+00	0.99776
85	3.7349E+13	1.28029E+00	0.53200
86	3.6528E+13	1.57210E+00	0.99895
87	8.0000E+12	1.13456E+00	0.99988
88	9.5769E+13	6.17087E+00	1.00000
89	3.0883E+10	2.45305E+00	0.99824
90	3.8937E+12	-5.39477E-02	0.97971
91	1.8000E+12	1.76372E+01	0.99919
92	7.8000E+11	9.76281E-05	1.00000
93	8.9868E+10	2.01130E+01	0.99999
94	6.9886E+12	7.65984E+00	0.91428
95	1.9984E+15	-3.32238E+01	0.84868
96	6.0163E+00	-1.13822E-04	0.73488
97	4.4292E+15	2.14502E-05	0.99307
98	1.7945E+01	2.16902E-05	0.67666
99	9.1136E-02	2.16023E-05	0.99195
100	2.5679E+08	5.46673E-10	0.99985
101	1.1365E+13	1.48680E-06	0.81714
102	1.0504E+11	1.84693E-07	0.98774
103	1.6608E+11	-5.09767E-04	0.99802
104	1.2000E+13	1.04024E-09	1.00000
105	3.8011E+13	-2.76070E-06	0.99592
106	5.9286E+12	9.88959E-03	0.62446
107	6.9362E+12	5.21894E-02	0.99524
108	2.3378E+13	9.24716E-04	0.98632
109	3.7000E+12	-9.31316E-04	1.00000
110	2.0000E+13	2.89274E-05	1.00000
111	1.0000E+13	1.32673E-10	1.00000
112	2.0000E+13	4.29779E-05	0.99338
113	7.0618E+11	1.35350E-11	0.99990
114	2.0000E+12	3.83195E-11	0.99956
115	1.0685E+13	1.13530E-03	0.99995
116	2.4276E+12	1.60201E+00	0.98681
117	8.2936E+12	1.71995E-02	0.92047
118	8.0889E+15	-6.39344E-01	0.99936
119	2.1873E+14	7.37043E-01	1.00000
120	3.5248E+07	-8.45191E-08	0.35304
121	1.3944E+07	-1.13540E-03	0.99996
122	7.2356E+03	1.59753E-06	0.65265
123	4.0000E+12	8.25612E-08	1.00000
124	9.2424E+06	-1.50490E-04	0.97148
125	1.5129E+10	-1.15446E-05	0.99977
126	1.6196E+10	2.68156E-09	0.94538
127	6.6303E+11	1.31456E-07	0.75694
128	2.6693E+09	1.11070E-02	0.99999
129	9.8902E+15	5.25262E-08	0.00084
130	9.5491E+15	-1.10940E-02	0.87002
131	5.0000E+12	-3.19520E-07	0.68548
132	6.5192E+15	1.34555E-05	0.02727
133	3.6000E+13	1.76069E-06	0.72745

DERIVATIVES (CGS UNITS): T 1.94923E+05 RHO 8.54162E-02
MIXTURE MOLECULAR WEIGHT 26.63512 TOTAL ENERGY EXCHANGE RATE -9.14644E+07 MASS FRACTION SUM 1.00000000
(CAL-CM**3/GM**2/SEC)

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 2.699986E-01 S UP TO THIS TIME - 1.477000E+01 S

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS - 190
TOTAL NO. OF DERIVATIVE EVALUATIONS - 232
TOTAL NO. OF JACOBIAN EVALUATIONS - 28
TOTAL CPU TIME - 14.769997 S

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 18.459999 S

(LSENS) READ DATA FOR NEXT CASE

TABLE D.2.—Continued.
(f) Case 6

DISTANCE-PRESSURE VERSION			LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM					NASA LEWIS RESEARCH CENTER		
			LEWIS	METHANE	AIR	MECHANISM	CONSTANT PRESSURE FLOW PROBLEM	CASE 6		
REACTION NUMBER			REACTION				REACTION RATE VARIABLES		ACTIVATION ENERGY	
							A	N		
1	M	+	1*CH4	=	1*CH3	+	1*H	2.00000E+17	0.0000	88000.00
2	1*H	+	1*CH4	=	1*CH3	+	1*H2	1.26000E+14	0.0000	11900.00
3	1*CH4	+	1*O2	=	1*CH3	+	1*H2O	7.94000E+13	0.0000	56000.00
4	1*O	+	1*CH4	=	1*CH3	+	1*H	1.90000E+14	0.0000	11720.00
5	1*OH	+	1*CH4	=	1*CH3	+	1*H2O	2.50000E+13	0.0000	5010.00
6	1*CH3	+	1*O2	=	1*CH3O	+	1*O	2.40000E+13	0.0000	28680.00
7	1*CH3	+	1*OH	=	1*CH3O	+	1*H	6.30000E+12	0.0000	0.00
8	M	+	1*CH3O	=	1*CH2O	+	1*H	5.00000E+13	0.0000	21000.00
9			2*CH3	=	1*C2H6	+	1*H	2.40000E+14	-0.4000	0.00
10	1*H	+	1*C2H6	=	1*C2H5	+	1*H2	1.32000E+14	0.0000	9700.00
11	1*O	+	1*C2H6	=	1*C2H5	+	1*OH	1.13000E+14	0.0000	7850.00
12	1*OH	+	1*C2H6	=	1*C2H5	+	1*H2O	8.70000E+13	0.0000	3520.00
13	M	+	1*C2H5	=	1*C2H4	+	1*H	1.00000E+17	0.0000	31000.00
14	1*C2H5	+	1*O2	=	1*C2H4	+	1*H2O	2.00000E+12	0.0000	5000.00
15	1*H	+	1*C2H5	=	1*C2H4	+	1*H2	4.80000E+13	0.0000	0.00
16	1*CH3	+	1*CH2	=	1*C2H4	+	1*H	2.00000E+13	0.0000	0.00
17	1*H	+	1*C2H4	=	1*H2	+	1*C2H3	1.50000E+14	0.0000	10200.00
18	M	+	1*C2H4	=	1*C2H2	+	1*H2	2.60000E+17	0.0000	79300.00
19	1*C2H4	+	1*OH	=	1*C2H3	+	1*H2O	4.80000E+12	0.0000	1230.00
20	1*C2H4	+	1*OH	=	1*CH3	+	1*CH2O	2.00000E+12	0.0000	960.00
21	1*C2H4	+	1*O	=	1*CH3	+	1*HCO	3.30000E+12	0.0000	1130.00
22	1*C2H4	+	1*O	=	1*CH2O	+	1*CH2	2.50000E+13	0.0000	5000.00
23	M	+	1*C2H3	=	1*C2H2	+	1*H	3.00000E+15	0.0000	32000.00
24	1*C2H3	+	1*O2	=	1*CH2O	+	1*HCO	3.98000E+12	0.0000	-250.00
25	1*C2H3	+	1*H	=	1*C2H2	+	1*H2	6.00000E+12	0.0000	0.00
26	1*C2H3	+	1*O	=	1*C2H2O	+	1*H	3.30000E+13	0.0000	0.00
27	1*C2H3	+	1*OH	=	1*C2H2	+	1*H2O	5.00000E+12	0.0000	0.00
28	1*C2H3	+	1*CH2	=	1*C2H2	+	1*CH3	5.00000E+13	0.0000	0.00
29	1*C2H3	+	1*CH2	=	2*CH2	+	1*H	3.00000E+13	0.0000	0.00
30	M	+	1*C2H2	=	1*CH2	+	1*H	4.20000E+16	0.0000	107000.00
31	1*C2H2	+	1*O	=	1*CH2	+	1*CO	1.60000E+14	0.0000	9890.00
32	1*C2H2	+	1*O	=	1*C2HO	+	1*H	6.00000E+14	0.0000	10640.00
33	1*C2H2	+	1*OH	=	1*CH2	+	1*H2O	6.30000E+12	0.0000	7000.00
34	1*C2H2	+	1*OH	=	1*C2H2O	+	1*H	3.20000E+11	0.0000	200.00
35	1*C2H	+	1*O2	=	1*C2HO	+	1*O	5.00000E+13	0.0000	1500.00
36	1*C2H	+	1*OH	=	1*C2HO	+	1*H	2.00000E+13	0.0000	0.00
37	1*C2HO	+	1*O2	=	2*CO	+	1*OH	1.46000E+12	0.0000	2500.00
38	1*C2HO	+	1*O	=	2*CO	+	1*H	1.20200E+12	0.0000	0.00
39	1*C2HO	+	1*OH	=	2*HCO	+	1*H	1.00000E+13	0.0000	0.00
40	1*C2HO	+	1*H	=	1*CH2	+	1*CO	5.00000E+13	0.0000	0.00
41	1*C2HO	+	1*CH2	=	1*CH2H3	+	1*CO	3.00000E+13	0.0000	0.00
42	1*C2HO	+	1*CH2	=	1*CH2O	+	1*C2H	1.00000E+13	0.0000	2000.00
43			2*C2HO	=	1*C2H2	+	2*CO	1.00000E+13	0.0000	0.00
44	1*C2H2O	+	1*OH	=	1*CH2O	+	1*HCO	2.80000E+13	0.0000	0.00
45	1*C2H2O	+	1*OH	=	1*C2HO	+	1*H2O	7.50000E+12	0.0000	3000.00
46	1*C2H2O	+	1*H	=	1*CH3	+	1*CO	1.13000E+13	0.0000	3428.00
47	1*C2H2O	+	1*H	=	1*C2HO	+	1*H2	7.50000E+13	0.0000	8000.00
48	1*C2H2O	+	1*O	=	1*C2HO	+	1*OH	5.00000E+13	0.0000	8000.00
49	1*C2H2O	+	1*O	=	1*CH2O	+	1*CO	2.00000E+13	0.0000	0.00
50	M	+	1*C2H2O	=	1*CH2	+	1*CO	2.00000E+16	0.0000	60000.00
51	1*CH2H	+	1*O	=	1*CO	+	1*CH	5.00000E+13	0.0000	0.00
52	1*CH3O	+	1*O2	=	1*CH2O	+	1*H2O	1.00000E+13	0.0000	1770.00
53	1*CH3O	+	1*H	=	1*CH2O	+	1*H2	2.00000E+13	0.0000	0.00
54	M	+	1*CH2O	=	1*HCO	+	1*H	5.00000E+16	0.0000	81000.00
55	1*CH2O	+	1*OH	=	1*HCO	+	1*H2O	3.00000E+13	0.0000	1200.00
56	1*CH2O	+	1*H	=	1*HCO	+	1*H2	2.50000E+13	0.0000	3990.00
57	1*CH2O	+	1*O	=	1*HCO	+	1*OH	3.50000E+13	0.0000	3510.00
58	1*CH3	+	1*CH2O	=	1*CH4	+	1*HCO	1.00000E+10	0.5000	6000.00
59	1*CH3	+	1*HCO	=	1*CH4	+	1*CO	3.00000E+11	0.5000	0.00
60	1*CH3	+	1*H2O	=	1*CH3O	+	1*OH	2.00000E+13	0.0000	0.00
61	M	+	1*CH3	=	1*CH2	+	1*H	1.95000E+16	0.0000	91600.00
62	1*H	+	1*CH3	=	1*H2	+	1*CH2	2.70000E+11	0.6700	25700.00
63	1*O	+	1*CH3	=	1*OH	+	1*CH2	1.90000E+11	0.6800	25700.00
64	1*OH	+	1*CH3	=	1*H2O	+	1*CH2	2.70000E+11	0.6700	25700.00
65	1*CH	+	1*CO2	=	1*HCO	+	1*CO	3.70000E+12	0.0000	0.00
66	1*CH	+	1*O2	=	1*HCO	+	1*O	1.00000E+13	0.0000	0.00
67	1*CH2	+	1*O2	=	1*CH2O	+	1*O	5.00000E+11	0.5000	6460.00
68	1*CH2	+	1*O	=	1*CH	+	1*OH	2.00000E+11	0.7000	25800.00
69	1*CH2	+	1*OH	=	1*CH	+	1*H2O	5.00000E+11	0.5000	5900.00
70	1*CH2	+	1*H	=	1*CH	+	1*H2	3.20000E+11	0.7000	4970.00
71	M	+	2*CH2	=	1*C2H3	+	1*H	5.00000E+12	0.0000	0.00
72			2*CH2	=	1*C2H2	+	1*H2	4.00000E+13	0.0000	0.00
73	1*HCO	+	1*O2	=	1*CO	+	1*H2O	3.00000E+13	0.0000	0.00
74	1*HCO	+	1*O	=	1*CO	+	1*OH	3.00000E+13	0.0000	0.00
75	1*HCO	+	1*OH	=	1*CO	+	1*H2O	3.00000E+13	0.0000	0.00
76	1*HCO	+	1*H	=	1*CO	+	1*H2	2.00000E+13	0.0000	0.00
77	M	+	1*HCO	=	1*H	+	1*CO	2.90000E+14	0.0000	15570.00
78	1*CO	+	1*O	=	1*CO2	+	M	2.40000E+15	0.0000	4100.00
79	1*CO	+	1*O2	=	1*CO2	+	1*O	2.50000E+12	0.0000	47690.00
80	1*CO	+	1*OH	=	1*CO2	+	1*H	4.17000E+11	0.0000	1800.00
81	1*CO	+	1*H2O	=	1*CO2	+	1*OH	5.75000E+13	0.0000	22930.00
82	1*O	+	1*H2O	=	2*OH	+	1*O	6.80000E+13	0.0000	18365.00
83	1*H	+	1*O2	=	1*OH	+	1*O	1.80000E+14	0.0000	16400.00
84	1*O	+	1*H2	=	1*OH	+	1*H	4.20000E+14	0.0000	13750.00
85	1*H	+	1*H2O2	=	1*H2	+	1*O2	7.28000E+13	0.0000	2126.00
86	1*O	+	1*H2O2	=	1*OH	+	1*O2	5.00000E+13	0.0000	1000.00
87	1*H2O2	+	1*OH	=	1*H2O	+	1*O2	8.00000E+12	0.0000	0.00
88	1*H	+	1*H2O2	=	2*OH	+	1*H	1.34000E+14	0.0000	1070.00
89	1*H2	+	1*H2O2	=	1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00
90	1*OH	+	1*H2O2	=	1*H2O	+	1*H2O2	6.10000E+12	0.0000	1430.00
91			2*H2O2	=	1*H2O2	+	1*O2	1.80000E+12	0.0000	0.00
92	1*H	+	1*H2O2	=	1*OH	+	1*H2O	7.80000E+11	0.0000	0.00
93	M	+	1*H2O2	=	2*OH	+	1.44000E+17	0.0000	45510.00	
94	1*H2	+	1*OH	=	1*H2O	+	1*H	4.74000E+13	0.0000	6098.00
95	1*H	+	1*O2	=	1*H2O2	+	M	1.46000E+15	0.0000	1000.00
96	M	+	1*H2O	=	1*H	+	1*OH	1.30000E+15	0.0000	105140.00
97	1*H	+	1*O	=	1*OH	+	H	7.10000E+18	-1.0000	0.00
98	M	+	1*H2	=	2*H	+	1*H	2.20000E+14	0.0000	96000.00
99	M	+	1*O2	=	2*O	+	1*H	1.80000E+18	1.0000	118020.00
100	1*CH	+	1*H2	=	1*CHN	+	1*H	1.00000E+11	0.0000	13000.00
101	1*CH	+	1*H2	=	1*CHN	+	1*H	6.00000E+13	0.0000	5500.00
102	1*O	+	1*CHN	=	1*OH	+	1*CH	1.40000E+11	0.6800	16900.00

TABLE D.2.—Continued.
(f) Continued.

103	1*OH	+	1*HCH	=	1*HHCO	+	1*H	4.00000E+11	0.0000	2800.00
104	1*CH	+	1*O	=	1*CO	+	1*H	1.20000E+13	0.0000	0.00
105	1*CH	+	1*OH	=	1*HCO	+	1*H	2.50000E+14	0.0000	6000.00
106	1*H2	+	1*HCO	=	1*HHCO	+	1*H	1.00000E+14	0.0000	9000.00
107	1*HHCO	+	1*H	=	1*HH2	+	1*O	1.00000E+14	0.0000	8500.00
108	1*CH	+	1*O2	=	1*HCO	+	1*O	3.20000E+13	0.0000	1000.00
109	1*CH	+	1*CO2	=	1*HCO	+	1*CO	3.70000E+12	0.0000	0.00
110	1*O	+	1*HCO	=	1*HO	+	1*CO	2.00000E+13	0.0000	0.00
111	1*H	+	1*HCO	=	1*H2	+	1*CO	1.00000E+13	0.0000	0.00
112	1*H	+	1*HCO	=	1*HH	+	1*CO	2.00000E+13	0.0000	0.00
113	1*CH	+	1*HO	=	1*H	+	1*HCO	1.60000E+13	0.0000	9940.00
114	1*CH	+	1*HO	=	1*O	+	1*HCH	2.00000E+12	0.0000	0.00
115	1*HH	+	1*HO	=	1*H	+	1*H2O	5.00000E+11	0.5000	2000.00
116	1*HO2	+	1*HO	=	1*HO2	+	1*OH	2.09000E+12	0.0000	-477.00
117	1*O	+	1*HO2	=	1*HO	+	1*O2	1.00000E+13	0.0000	596.00
118	1*HO	+	1*H	=	1*HO	+	H	5.62000E+15	0.0000	-1160.00
119	1*HO2	+	1*H	=	1*H	+	1*OH	3.47000E+14	0.0000	1470.00
120	1*HO	+	1*O	=	1*H	+	1*OH	2.63000E+14	0.0000	50410.00
121	1*HO	+	1*O	=	1*H	+	1*O2	3.80000E+09	1.0000	41370.00
122	1*O	+	1*H2	=	1*HO	+	1*H	1.80000E+14	0.0000	76250.00
123	1*H	+	1*HO2	=	2*HO	+	1*H	4.00000E+12	0.0000	0.00
124	H	+	1*HO2	=	1*H2	+	1*O	6.92000E+23	-2.5000	65000.00
125	1*O	+	1*HO2	=	1*H2	+	1*O2	1.00000E+14	0.0000	28020.00
126	1*O	+	1*H2O	=	2*HO	+	1*O	6.92000E+13	0.0000	26630.00
127	1*H2O	+	1*H	=	1*H2	+	1*OH	7.59000E+13	0.0000	15100.00
128	1*HO2	+	1*H2	=	1*HHO2	+	1*H	2.40000E+13	0.0000	29000.00
129	1*OH	+	1*HO2	=	1*HHO3	+	H	3.00000E+15	0.0000	-3800.00
130	1*OH	+	1*HO	=	1*HHO2	+	H	5.60000E+15	0.0000	-1700.00
131	1*HHO	+	1*H	=	1*H2	+	1*HO	5.00000E+12	0.0000	0.00
132	1*H	+	1*HO	=	1*HHO	+	H	5.40000E+15	0.0000	-600.00
133	1*HHO	+	1*OH	=	1*H2O	+	1*HO	3.60000E+13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	, 93) =	2.30000	M(O2	, 93) =	0.78000	M(H2O	, 93) =	6.00000	M(H2O2	, 93) =	6.60000
M(O2	, 95) =	1.30000	M(H2	, 95) =	1.30000	M(H2O	, 95) =	21.30000	M(O2	, 95) =	7.00000
M(H2	, 96) =	4.00000	M(O2	, 96) =	1.50000	M(H2O	, 96) =	20.00000	M(H2	, 96) =	1.50000
M(CO2	, 96) =	4.00000	M(H2	, 98) =	4.10000	M(O2	, 98) =	2.00000	M(H2O	, 98) =	15.00000
M(H2	, 98) =	2.00000	M(O2	, 129) =	0.70000	M(H2	, 129) =	1.40000			

*** EQUILIBRIUM CALCULATION ***

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED ENTHALPY AND PRESSURE

	INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE (ATM)	1.7300	1.7300	1.0000
VELOCITY (CM/SEC)	0.00	0.00	1.0000
DENSITY (G/CM**3)	3.49869E-04	2.30793E-04	0.6597
TEMPERATURE (DEG K)	1700.00	2553.11	1.5018
ENTHALPY (CAL/G)	379.22696	379.22711	1.00000
INTERNAL ENERGY (CAL/G)	259.48010	197.69731	0.76190
SP. HEAT (CP) (CAL/G/DEG K)	0.32691	0.54085	1.65441
ENTROPY (CAL/G/DEG K)	2.1420	2.3097	1.0783
MACH NUMBER	0.0000	0.0000	1.0000
GAMMA	1.2746	1.1514	0.9033
SONIC VELOCITY (CM/SEC)	79913.95	94814.24	1.1865

SPECIES	MOLE FRACTION
CH4	2.79483E-10
CH3	2.79483E-10
H	1.00214E-03
H2	1.76022E-03
O2	8.94256E-02
HO2	1.55944E-05
O	4.23158E-03
OH	1.15976E-02
H2O	9.05405E-02
CH3O	2.79483E-10
CH2O	2.79483E-10
C2H6	2.79483E-10
C2H5	2.79483E-10
C2H4	2.79483E-10
CH2	2.79483E-10
C2H3	2.79483E-10
C2H2	2.79483E-10
HCO	2.79483E-10
C2H2O	2.79483E-10
C2H	2.79483E-10
CO	5.35472E-03
C2HO	2.79483E-10
CH	2.79483E-10
CO2	4.39498E-02
H2O2	2.72872E-07
H2	7.36205E-01
HCM	2.79483E-10

TABLE D.2.—Continued.
(f) Continued.

	N	3.06077E-07
	CN	2.79483E-10
	HNCO	2.79483E-10
	NCO	2.79483E-10
	NH2	2.79483E-10
	NO	1.59036E-02
	NH	4.66032E-08
	NO2	1.16681E-05
	N2O	1.13359E-06
	HNO2	2.41994E-07
	HNO3	2.79483E-10
	HNO	3.58947E-07
MIXTURE MOLECULAR WEIGHT		27.94827
D(LOG VOLUME)/D(LOG T) AT CONSTANT P		1.0999
D(LOG VOLUME)/D(LOG P) AT CONSTANT T		-1.0039

COMPUTATIONAL WORK REQUIRED FOR EQUILIBRIUM CALCULATION:
NO. OF ITERATIONS = 15 CPU TIME = 7.999992E-02 S

** INITIAL CONDITIONS **

TIME	0.00000E+00	SEC	AREA	1.00000E+03	SQ CM	AXIAL POSITION	0.00000E+00	CM
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FLOW PROPERTIES

PRESSURE (ATM)	1.73000
VELOCITY (CM/SEC)	159827.88
DENSITY (G/CM**3)	3.49869E-04
TEMPERATURE (DEG K)	1700.00
MASS FLOW RATE (G/SEC)	5.59188E+04
ENTROPY (CAL/G/DEG K)	2.1420
MACH NUMBER	2.0000
GAMMA	1.2746
ENTHALPY (CAL/G)	3.79227E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.26913E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	FATE CONST (G/SEC)	NET ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	NET RATE/POSI- TIVE DIR RATE
CH4	6.17216E-07	4.97680E-02	-1.50903E-05	1	9.7244E+05	6.37423E+06	1.00000
CH3	0.00000E+00	0.00000E+00	1.50903E-05	2	3.7198E+12	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	7.44369E-06	3	5.0180E+06	3.32443E+06	1.00000
H2	0.00000E+00	0.00000E+00	0.00000E+00	4	5.9162E+12	0.00000E+00	0.00000
O2	2.46886E-06	1.99072E-01	-8.05210E-05	5	5.6736E+12	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	7.64658E-06	6	4.9334E+09	0.00000E+00	0.00000
O	0.00000E+00	0.00000E+00	7.28745E-05	7	6.3000E+12	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	0.00000E+00	8	9.9825E+10	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	9	1.2247E+13	0.00000E+00	0.00000
CH3O	0.00000E+00	0.00000E+00	0.00000E+00	10	7.4740E+12	0.00000E+00	0.00000
CH2O	0.00000E+00	0.00000E+00	0.00000E+00	11	1.1064E+13	0.00000E+00	0.00000
C2H6	0.00000E+00	0.00000E+00	0.00000E+00	12	3.0690E+13	0.00000E+00	0.00000
C2H5	0.00000E+00	0.00000E+00	0.00000E+00	13	1.0344E+13	0.00000E+00	0.00000
C2H4	0.00000E+00	0.00000E+00	0.00000E+00	14	4.5524E+11	0.00000E+00	0.00000
CH2	0.00000E+00	0.00000E+00	0.00000E+00	15	4.8000E+13	0.00000E+00	0.00000
C2H3	0.00000E+00	0.00000E+00	0.00000E+00	16	2.0000E+13	0.00000E+00	0.00000
C2H2	0.00000E+00	0.00000E+00	0.00000E+00	17	7.3247E+12	0.00000E+00	0.00000
HCO	0.00000E+00	0.00000E+00	0.00000E+00	18	1.6606E+07	0.00000E+00	0.00000
C2H2O	0.00000E+00	0.00000E+00	0.00000E+00	19	3.3351E+12	0.00000E+00	0.00000
C2H	0.00000E+00	0.00000E+00	0.00000E+00	20	1.5053E+12	0.00000E+00	0.00000
CO	0.00000E+00	0.00000E+00	0.00000E+00	21	2.3618E+12	0.00000E+00	0.00000
C2HO	0.00000E+00	0.00000E+00	0.00000E+00	22	5.6904E+12	0.00000E+00	0.00000
CH	0.00000E+00	0.00000E+00	0.00000E+00	23	2.3080E+11	0.00000E+00	0.00000
CO2	0.00000E+00	0.00000E+00	0.00000E+00	24	4.2857E+12	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	25	6.0000E+12	0.00000E+00	0.00000

TABLE D.2.—Continued.
(f) Continued.

H2	9.31578E-06	7.51160E-01	-1.20855E-11	26	3.3000E+13	0.00000E+00	0.00000
HCN	0.00000E+00	0.00000E+00	0.00000E+00	27	5.0000E+12	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	0.00000E+00	28	3.0000E+13	0.00000E+00	0.00000
CH	1.24019E-12	1.00000E-07	-7.28744E-05	29	3.0000E+13	0.00000E+00	0.00000
HNCO	0.00000E+00	0.00000E+00	0.00000E+00	30	7.3700E+02	0.00000E+00	0.00000
HCO	0.00000E+00	0.00000E+00	7.28744E-05	31	8.5640E+12	0.00000E+00	0.00000
NH2	0.00000E+00	0.00000E+00	0.00000E+00	32	1.7044E+13	0.00000E+00	0.00000
NO	0.00000E+00	0.00000E+00	0.00000E+00	33	7.9329E+11	0.00000E+00	0.00000
NH	0.00000E+00	0.00000E+00	0.00000E+00	34	3.0160E+11	0.00000E+00	0.00000
HU2	0.00000E+00	0.00000E+00	0.00000E+00	35	3.2072E+13	0.00000E+00	0.00000
N2O	0.00000E+00	0.00000E+00	1.20855E-11	36	2.0000E+13	0.00000E+00	0.00000
HNH2	0.00000E+00	0.00000E+00	0.00000E+00	37	6.9656E+11	0.00000E+00	0.00000
HNH3	0.00000E+00	0.00000E+00	0.00000E+00	38	1.2020E+12	0.00000E+00	0.00000
HNH	0.00000E+00	0.00000E+00	0.00000E+00	39	1.0000E+13	0.00000E+00	0.00000
				40	5.0000E+13	0.00000E+00	0.00000
				41	3.0000E+13	0.00000E+00	0.00000
				42	5.5320E+12	0.00000E+00	0.00000
				43	1.0000E+13	0.00000E+00	0.00000
				44	2.8000E+13	0.00000E+00	0.00000
				45	3.0859E+12	0.00000E+00	0.00000
				46	4.0962E+12	0.00000E+00	0.00000
				47	7.0241E+12	0.00000E+00	0.00000
				48	4.6827E+12	0.00000E+00	0.00000
				49	2.0000E+13	0.00000E+00	0.00000
				50	3.8682E+08	0.00000E+00	0.00000
				51	5.0000E+13	0.00000E+00	0.00000
				52	1.1974E+12	0.00000E+00	0.00000
				53	2.0000E+13	0.00000E+00	0.00000
				54	9.9307E+06	0.00000E+00	0.00000
				55	2.1031E+13	0.00000E+00	0.00000
				56	7.6735E+12	0.00000E+00	0.00000
				57	1.2383E+13	0.00000E+00	0.00000
				58	6.9803E+10	0.00000E+00	0.00000
				59	1.2369E+13	0.00000E+00	0.00000
				60	2.0000E+13	0.00000E+00	0.00000
				61	3.2643E+06	0.00000E+00	0.00000
				62	1.9580E+10	0.00000E+00	0.00000
				63	1.4842E+10	0.00000E+00	0.00000
				64	1.9580E+10	0.00000E+00	0.00000
				65	3.7000E+12	0.00000E+00	0.00000
				66	1.0000E+13	0.00000E+00	0.00000
				67	2.6268E+12	0.00000E+00	0.00000
				68	1.7601E+10	0.00000E+00	0.00000
				69	3.5950E+12	0.00000E+00	0.00000
				70	1.3413E+13	0.00000E+00	0.00000
				71	5.0000E+12	0.00000E+00	0.00000
				72	4.0000E+13	0.00000E+00	0.00000
				73	3.0000E+13	0.00000E+00	0.00000
				74	3.0000E+13	0.00000E+00	0.00000
				75	3.0000E+13	0.00000E+00	0.00000
				76	2.0000E+13	0.00000E+00	0.00000
				77	2.8889E+12	0.00000E+00	0.00000
				78	7.1305E+14	0.00000E+00	0.00000
				79	1.8492E+06	0.00000E+00	0.00000
				80	3.1015E+11	0.00000E+00	0.00000
				81	6.4836E+10	0.00000E+00	0.00000
				82	2.9616E+11	0.00000E+00	0.00000
				83	1.4726E+12	0.00000E+00	0.00000
				84	7.1708E+12	0.00000E+00	0.00000
				85	3.8799E+13	0.00000E+00	0.00000
				86	3.7189E+13	0.00000E+00	0.00000
				87	8.0000E+12	0.00000E+00	0.00000
				88	9.7622E+13	0.00000E+00	0.00000
				89	4.8329E+10	0.00000E+00	0.00000
				90	3.9948E+12	0.00000E+00	0.00000
				91	1.8000E+12	0.00000E+00	0.00000
				92	7.8000E+11	0.00000E+00	0.00000
				93	2.0307E+11	0.00000E+00	0.00000
				94	7.7952E+12	0.00000E+00	0.00000
				95	1.9630E+15	0.00000E+00	0.00000
				96	3.9562E+01	0.00000E+00	0.00000
				97	4.1765E+15	0.00000E+00	0.00000
				98	1.0018E+02	0.00000E+00	0.00000
				99	7.1175E-01	2.12950E+01	1.00000
				100	3.6090E+08	0.00000E+00	0.00000
				101	1.2497E+13	0.00000E+00	0.00000
				102	1.4798E+11	0.00000E+00	0.00000
				103	1.7462E+11	0.00000E+00	0.00000
				104	1.2000E+13	0.00000E+00	0.00000
				105	4.2324E+13	0.00000E+00	0.00000
				106	6.9658E+12	0.00000E+00	0.00000
				107	8.0770E+12	0.00000E+00	0.00000
				108	2.3801E+13	-3.77764E+06	1.00000
				109	3.7000E+12	0.00000E+00	0.00000
				110	2.0000E+13	0.00000E+00	0.00000
				111	1.0000E+13	0.00000E+00	0.00000
				112	2.0000E+13	0.00000E+00	0.00000
				113	8.4381E+11	0.00000E+00	0.00000
				114	2.0000E+12	0.00000E+00	0.00000
				115	1.1405E+13	0.00000E+00	0.00000
				116	2.4070E+12	0.00000E+00	0.00000
				117	8.3826E+12	0.00000E+00	0.00000
				118	7.9225E+15	0.00000E+00	0.00000
				119	2.2457E+14	0.00000E+00	0.00000
				120	8.6958E+07	0.00000E+00	0.00000
				121	3.1028E+07	0.00000E+00	0.00000
				122	2.8358E+04	0.00000E+00	0.00000
				123	4.0000E+12	0.00000E+00	0.00000
				124	2.5566E+07	0.00000E+00	0.00000
				125	2.4991E+10	7.80528E+00	1.00000
				126	2.6097E+10	0.00000E+00	0.00000
				127	8.6897E+11	0.00000E+00	0.00000
				128	4.4875E+09	0.00000E+00	0.00000
				129	9.2394E+15	0.00000E+00	0.00000
				130	9.2627E+15	0.00000E+00	0.00000
				131	5.0000E+12	0.00000E+00	0.00000
				132	6.4495E+15	0.00000E+00	0.00000
				133	3.6000E+13	0.00000E+00	0.00000
DERIVATIVES (CGS UNITS): T	-5.12217E-02	RHO	9.22781E-09	V	0.00000E+00		
MIXTURE MOLECULAR WEIGHT	28.21102	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	5.92105E+06	MASS FRACTION SUM	1.00000000		
CPU TIME FOR INITIALIZATION OF LSENS =	2.340000	S					

TABLE D.2.—Continued.
(f) Continued.

TIME 2.94066E-04 SEC		AREA 1.43983E+03 SQ CM		AXIAL POSITION 4.70000E+01 CM			
FLOW PROPERTIES				INTEGRATION INDICATORS			
PRESSURE 1.73000 (ATM)				STEPS FROM LAST PRINT	4		
VELOCITY 159827.88 (CM/SEC)				AVERAGE STEP SIZE	0.26316E+00		
DENSITY 2.42993E-04 (G/CM**3)				METHOD ORDER	3		
TEMPERATURE 2389.90 (DEG K)				TOTAL NUMBER OF STEPS	187		
MASS FLOW RATE 5.59188E+04 (G/SEC)				FUNCT EVALUATIONS	284		
ENTROPY 2.3063 (CAL/G/DEG K)				JACOBIAN EVALUATIONS	36		
MACH NUMBER 1.6673							
GAMMA 1.2738							
ENTHALPY 3.79227E+02 (CAL/G)							
SP. HEAT (CP) 3.35630E-01 (CAL/G/DEG K)							
CHEMICAL PROPERTIES							
SPECIES	CONCENTRATION (MOL/L/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOL/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL/CM**3/G**1/2/SEC)	NET RATE/POSITIVE DIR RATE
CH4	5.73493E-11	6.50081E-06	-5.57743E-06	1	1.7933E+09	-5.21884E+07	0.97006
CH3	1.12913E-09	1.27992E-04	-1.14166E-04	2	1.0284E+13	4.49566E+04	0.17311
H	4.22012E-08	4.78370E-03	-5.23454E-04	3	6.0086E+08	-7.63059E+04	0.74010
H2	3.80903E-08	4.31771E-03	-2.30715E-04	4	1.6106E+13	7.46885E+05	0.17599
H2	8.62787E-07	9.78009E-02	-1.05454E-03	5	8.7054E+12	-3.18369E+06	0.17575
H2O	1.73505E-10	1.96676E-05	-5.68861E-07	6	5.7214E+10	1.16487E+06	0.04310
O	1.08953E-07	1.23503E-02	-8.58925E-04	7	6.3000E+12	8.81381E+06	0.04144
OH	1.48846E-07	1.68724E-02	-1.29853E-04	8	6.0059E+11	1.14117E+07	1.00000
H2O	7.21783E-07	8.18173E-02	7.43665E-04	9	1.0687E+13	-1.11000E+06	0.05364
CH3O	6.20209E-12	7.03035E-07	-5.27733E-07	10	1.7121E+13	-5.38423E+03	0.99996
CH2O	1.76259E-11	1.99798E-06	-1.53116E-06	11	2.1638E+13	-1.22440E+04	0.99996
C2H6	7.14414E-14	8.09821E-09	6.99046E-08	12	4.1460E+13	-1.58056E+05	0.99996
C2H5	5.84465E-16	6.62517E-11	-2.64853E-09	13	1.4626E+14	4.30442E+05	0.87082
C2H4	3.3358E-13	3.77876E-08	-7.66669E-08	14	6.9790E+11	-7.57558E+01	0.98512
CH2	1.01723E-11	1.15308E-06	-9.92644E-07	15	4.8000E+13	-1.30923E+03	0.99680
C2H3	1.09283E-14	1.23877E-09	-1.52066E-09	16	2.0000E+13	-2.43183E+05	0.99901
C2H2	5.96399E-14	6.76045E-09	-1.78284E-08	17	1.7512E+13	-1.02700E+04	0.99919
HCO	1.07672E-12	1.22051E-07	-9.31583E-08	18	1.4561E+10	3.02366E+04	1.00000
C2H2O	1.72493E-14	1.95529E-09	-2.85693E-09	19	3.7048E+12	5.45364E+04	0.99920
C2H	3.48576E-16	3.95126E-11	-1.06144E-10	20	1.6340E+12	-2.00195E+04	0.99198
CO	1.31702E-07	1.49291E-02	-2.08396E-03	21	2.6012E+12	4.29343E+04	1.00000
CH	7.64025E-14	8.66057E-09	-2.00198E-08	22	8.7238E+12	-5.97272E+04	0.99997
CO	2.13501E-12	2.41787E-07	-2.17147E-07	23	3.5547E+12	2.55864E+05	0.99838
CO2	2.95745E-07	3.35241E-02	2.20719E-03	24	4.1951E+12	5.32165E+04	1.00000
H2O2	9.95871E-12	1.12886E-06	-1.64267E-07	25	6.0000E+12	-2.81409E+05	0.99996
H2	6.46972E-06	7.33373E-01	-1.37072E-05	26	3.5000E+13	-5.38937E+04	1.00000
HCN	3.49320E-13	3.95970E-08	-2.72924E-08	27	5.0000E+12	-1.05387E+04	0.99996
N	1.05796E-12	1.19924E-07	1.50385E-08	28	3.0000E+13	-3.66454E+00	0.99083
CH	2.25860E-15	2.56023E-10	-1.71786E-10	29	3.0000E+13	-1.60559E-06	0.99921
HNCO	5.03698E-14	5.70965E-09	-1.34140E-09	30	6.8926E+06	8.11258E+00	0.50947
HCO	1.49889E-14	1.69906E-09	-9.42490E-10	31	1.9939E+13	-1.04814E+05	0.99911
H2	2.28458E-12	2.58967E-07	9.42576E-09	32	4.2387E+13	-1.07208E+05	0.99317
NO	6.27721E-10	7.11550E-05	2.73613E-05	33	1.4428E+12	1.64036E+03	0.94969
NH	6.72476E-14	7.62282E-09	1.25351E-09	34	3.0680E+11	-1.03891E+03	0.86766
NO2	4.16756E-13	4.72411E-08	1.92319E-08	35	3.6459E+13	-5.01001E+03	0.86440
H2O	6.52489E-12	7.39626E-07	1.75917E-08	36	2.0000E+13	-7.28677E+02	1.00000
HNCO	2.64396E-14	2.99705E-09	7.54600E-10	37	8.6245E+11	-7.89664E+04	1.00000
HNCO	3.08559E-18	3.49766E-13	9.69517E-14	38	1.2020E+12	-1.67395E+04	1.00000
HNCO	8.95348E-14	1.01492E-08	1.93741E-09	39	1.0000E+13	-5.85659E+04	0.86955
				40	5.0000E+13	-5.75628E+01	0.99998
				41	3.0000E+13	-2.52975E+00	0.99994
				42	6.5630E+12	-7.47799E-02	1.00000
				43	1.0000E+13	-1.85277E+04	0.99986
				44	2.8000E+13	-1.33179E+03	0.44621
				45	3.9877E+12	3.41117E+04	0.93977
				46	5.4903E+12	-1.67974E+02	0.44644
				47	1.3915E+13	-4.43695E+01	1.00000
				48	9.2767E+12	-6.51035E+04	0.65841
				49	2.0000E+13	-2.35233E+03	0.99877
				50	6.5191E+10	-6.22748E+06	1.00000
				51	5.0000E+13	-7.42049E+06	1.00000
				52	2.2096E+12	4.61331E+05	0.99203
				53	2.0000E+13	-1.90304E+06	0.99980
				54	1.9577E+09	-6.59553E+06	0.99980
				55	2.3302E+13	-6.80754E+02	0.99976
				56	1.0791E+13	-2.69003E+04	0.99494
				57	1.6714E+13	-1.16626E+06	0.79507
				58	1.3820E+11	1.24817E+06	0.82368
				59	1.4666E+13	9.64434E+05	0.99563
				60	2.0000E+13	-2.54525E+06	0.99565
				61	8.1933E+07	-6.00556E+06	1.00000
				62	2.2115E+11	-2.24556E+07	1.00000
				63	1.6821E+11	-5.07638E+07	0.99999
				64	2.2115E+11	-2.07294E+03	0.93058
				65	3.7000E+12	-2.94060E+06	0.93056
				66	1.0000E+13	-4.31821E+05	0.93034
				67	5.6453E+12	-6.17280E+02	0.99982
				68	2.0256E+11	-9.14860E+03	1.00000
				69	7.0570E+12	1.68075E+07	0.98053
				70	2.6035E+13	-5.16700E+06	0.99583
				71	5.0000E+12	-8.42740E+06	0.99583
				72	4.0000E+13	-1.36281E+06	0.99582
				73	3.0000E+13	2.23351E+07	0.83103
				74	1.0122E+15	-2.71328E+08	0.98304
				75	1.0885E+08	-5.31123E+05	0.31387
				76	3.3782E+11	-8.71384E+08	0.31268
				77	4.6002E+11	-8.93220E+06	0.85306
				78	1.4226E+12	9.64819E+06	0.00030
				79	5.9803E+12	1.07360E+08	0.00174
				80	2.3219E+13	1.06120E+07	0.00348
				81	4.65281E+13	-2.38281E+08	0.78509
				82	4.0506E+13	-5.17051E+08	0.78584
				83	8.0000E+12	-1.85899E+08	0.78578

(f) **Concluded.**

DERIVATIVES (COS UNITS): T	2.14117E+01	RHD	-1.82533E-06	V	0.00000E+00	0.96280
MIXTURE MOLECULAR HEIGHT	27.54436	TOTAL ENERGY EXCHANGE RATE (CAL/CMH*1/2RGAZ/SEC)	-4.71681E+09	MASS FRACTION SUM	1.00000005	

COMPUTER TIME (CPU) REQUIRED, FOR THIS STEP - 3.800011E-01 S UP TO THIS TIME - 1.247001E+01 S

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM.

```

TOTAL NO. OF STEPS - 190
TOTAL NO. OF DERIVATIVE EVALUATIONS - 289
TOTAL NO. OF JACOBIAN EVALUATIONS - 37
TOTAL CPU TIME - 12.710009 S

```

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 21.950001 S

```
(LSENS)      READ DATA FOR NEXT CASE
```

MM DATA LINES MM

CC 1234567890¹1234567890²1234567890³1234567890⁴1234567890⁵1234567890⁶1234567890⁷1234567890⁸

LENS METHANE - AIR WITH AREA PROFILE OF CASE 6 CASE 7
REPEAT

```

REPEAT
DISTANCE AREA
$prob= false, combus= false,
xtb=0.10,0.20,0.25,0.30,0.32,0.34,0.36,0.37,0.38,0.39,0.40,0.41,0.
42,0.43,0.44,0.45,0.46,0.47,0.48,0.
mtb= 1000.00,1000.20,1004.65,1010.85,1023.22,1031.44,1042.92,1059.73,
1071.45,1087.06,1110.03,1133.75,1284.24,1350.79,1376.81,1397.15,
1414.00,1428.05,1439.83,1449.81,
$print=1023.22,1153.75,1439.83, &end
$start t=1700.0, mach=2.0, p=1.730, &end
CH4 0.049768
O2 0.199072
N2 0.75116
CN 0.0000001
END
$solver emax=5.0E-5, atolsp=1.0E-13, &end
FINIS

```

TABLE D.2.—Continued.
(g) Case 7

*** INITIAL CONDITIONS ***

TIME 0.00000E+00 SEC AREA 1.00000E+03 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE 1.73000
(ATM)
VELOCITY 159827.88
(CM/SEC)
DENSITY 3.49869E-04
(G/CM**3)
TEMPERATURE 1700.00
(DEG K)
MASS FLOW RATE 5.59188E+04
(G/SEC)
ENTROPY 2.1420
(CAL/G/DEG K)
MACH NUMBER 2.0000
GAMMA 1.2746
ENTHALPY 3.79227E+02
(CAL/G)
SP. HEAT (CP) 3.26913E-01
(CAL/G/DEG K)

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 0
AVERAGE STEP SIZE 0.00000E+00
METHOD ORDER 0
TOTAL NUMBER OF STEPS 0
FUNCT EVALUATIONS 0
JACOBIAN EVALUATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	NET RATE/POSI- TIVE DIR RATE
CH4	6.17216E-07	4.97680E-02	-1.50903E-05	1	9.7244E+05	6.37423E+06	1.00000
CH3	0.00000E+00	0.00000E+00	1.50903E-05	2	3.7198E+12	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	7.44369E-06	3	5.0180E+06	3.32443E+06	1.00000
H2	0.00000E+00	0.00000E+00	0.00000E+00	4	5.9162E+12	0.00000E+00	0.00000
O2	2.46886E-06	1.99072E-01	-8.05210E-05	5	5.6736E+12	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	7.64658E-06	6	4.9334E+09	0.00000E+00	0.00000
O	0.00000E+00	0.00000E+00	7.28745E-05	7	6.3000E+12	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	0.00000E+00	8	9.9825E+10	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	9	1.2247E+13	0.00000E+00	0.00000
CH3O	0.00000E+00	0.00000E+00	0.00000E+00	10	7.4740E+12	0.00000E+00	0.00000
CH2O	0.00000E+00	0.00000E+00	0.00000E+00	11	1.0644E+13	0.00000E+00	0.00000
C2H6	0.00000E+00	0.00000E+00	0.00000E+00	12	3.0690E+13	0.00000E+00	0.00000
C2H5	0.00000E+00	0.00000E+00	0.00000E+00	13	1.0344E+13	0.00000E+00	0.00000
C2H4	0.00000E+00	0.00000E+00	0.00000E+00	14	4.5524E+11	0.00000E+00	0.00000
CH2	0.00000E+00	0.00000E+00	0.00000E+00	15	4.8000E+13	0.00000E+00	0.00000
C2H3	0.00000E+00	0.00000E+00	0.00000E+00	16	2.0000E+13	0.00000E+00	0.00000
C2H2	0.00000E+00	0.00000E+00	0.00000E+00	17	7.3247E+12	0.00000E+00	0.00000
HCO	0.00000E+00	0.00000E+00	0.00000E+00	18	1.6606E+07	0.00000E+00	0.00000
C2H2O	0.00000E+00	0.00000E+00	0.00000E+00	19	3.3551E+12	0.00000E+00	0.00000
C2H	0.00000E+00	0.00000E+00	0.00000E+00	20	1.5053E+12	0.00000E+00	0.00000
CO	0.00000E+00	0.00000E+00	0.00000E+00	21	2.3618E+12	0.00000E+00	0.00000
C2HO	0.00000E+00	0.00000E+00	0.00000E+00	22	5.6904E+12	0.00000E+00	0.00000
CH	0.00000E+00	0.00000E+00	0.00000E+00	23	2.3080E+11	0.00000E+00	0.00000
CO2	0.00000E+00	0.00000E+00	0.00000E+00	24	4.2857E+12	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	25	6.0000E+12	0.00000E+00	0.00000
N2	9.31578E-06	7.51160E-01	-1.20855E-11	26	3.3000E+13	0.00000E+00	0.00000
HCN	0.00000E+00	0.00000E+00	0.00000E+00	27	5.0000E+12	0.00000E+00	0.00000
N	0.00000E+00	0.00000E+00	0.00000E+00	28	3.0000E+13	0.00000E+00	0.00000
CN	1.24019E-12	1.00000E-07	-7.28744E-05	29	5.0000E+13	0.00000E+00	0.00000
HNCO	0.00000E+00	0.00000E+00	0.00000E+00	30	7.3700E+02	0.00000E+00	0.00000
NCO	0.00000E+00	0.00000E+00	0.00000E+00	31	8.5640E+12	0.00000E+00	0.00000
NH2	0.00000E+00	0.00000E+00	7.28744E-05	32	1.7046E+13	0.00000E+00	0.00000
HO	0.00000E+00	0.00000E+00	0.00000E+00	33	7.9329E+11	0.00000E+00	0.00000
NH	0.00000E+00	0.00000E+00	0.00000E+00	34	3.0160E+11	0.00000E+00	0.00000
N2O	0.00000E+00	0.00000E+00	0.00000E+00	35	3.2072E+13	0.00000E+00	0.00000
N2O	0.00000E+00	0.00000E+00	1.20855E-11	36	2.0000E+13	0.00000E+00	0.00000
HNO2	0.00000E+00	0.00000E+00	0.00000E+00	37	6.9656E+11	0.00000E+00	0.00000
HNO3	0.00000E+00	0.00000E+00	0.00000E+00	38	1.2020E+12	0.00000E+00	0.00000
HNO	0.00000E+00	0.00000E+00	0.00000E+00	39	1.0000E+13	0.00000E+00	0.00000
				40	5.0000E+13	0.00000E+00	0.00000
				41	3.0000E+13	0.00000E+00	0.00000
				42	5.5320E+12	0.00000E+00	0.00000
				43	1.0000E+13	0.00000E+00	0.00000
				44	2.8000E+13	0.00000E+00	0.00000
				45	3.0859E+12	0.00000E+00	0.00000
				46	4.0962E+12	0.00000E+00	0.00000
				47	7.0241E+12	0.00000E+00	0.00000
				48	4.6827E+12	0.00000E+00	0.00000
				49	2.0000E+13	0.00000E+00	0.00000
				50	3.8682E+08	0.00000E+00	0.00000
				51	5.0000E+13	0.00000E+00	0.00000
				52	1.1974E+12	0.00000E+00	0.00000
				53	2.0000E+13	0.00000E+00	0.00000
				54	1.9307E+06	0.00000E+00	0.00000
				55	2.1031E+13	0.00000E+00	0.00000
				56	7.6735E+12	0.00000E+00	0.00000
				57	1.2383E+13	0.00000E+00	0.00000
				58	6.9803E+10	0.00000E+00	0.00000
				59	1.2369E+13	0.00000E+00	0.00000
				60	2.0000E+13	0.00000E+00	0.00000
				61	3.2663E+04	0.00000E+00	0.00000
				62	1.9580E+10	0.00000E+00	0.00000
				63	1.4842E+10	0.00000E+00	0.00000
				64	1.9580E+10	0.00000E+00	0.00000
				65	3.7000E+12	0.00000E+00	0.00000
				66	1.0000E+13	0.00000E+00	0.00000
				67	2.6268E+12	0.00000E+00	0.00000
				68	1.7601E+10	0.00000E+00	0.00000
				69	3.5950E+12	0.00000E+00	0.00000
				70	1.3413E+13	0.00000E+00	0.00000
				71	5.0000E+12	0.00000E+00	0.00000
				72	4.0000E+13	0.00000E+00	0.00000
				73	3.0000E+13	0.00000E+00	0.00000
				74	3.0000E+13	0.00000E+00	0.00000
				75	3.0000E+13	0.00000E+00	0.00000

TABLE D.2.—Continued.
(g) Continued.

76	2.0000E+13	0.0000E+00	0.00000
77	2.8889E+12	0.0000E+00	0.00000
78	7.1305E+14	0.0000E+00	0.00000
79	1.8492E+06	0.0000E+00	0.00000
80	3.1015E+11	0.0000E+00	0.00000
81	6.4836E+10	0.0000E+00	0.00000
82	2.9616E+11	0.0000E+00	0.00000
83	1.4726E+12	0.0000E+00	0.00000
84	7.1708E+12	0.0000E+00	0.00000
85	3.8799E+13	0.0000E+00	0.00000
86	3.7189E+13	0.0000E+00	0.00000
87	8.0000E+12	0.0000E+00	0.00000
88	9.7622E+13	0.0000E+00	0.00000
89	4.8329E+10	0.0000E+00	0.00000
90	3.9948E+12	0.0000E+00	0.00000
91	1.8000E+12	0.0000E+00	0.00000
92	7.8000E+11	0.0000E+00	0.00000
93	2.0307E+11	0.0000E+00	0.00000
94	7.7952E+12	0.0000E+00	0.00000
95	1.9630E+15	0.0000E+00	0.00000
96	3.9562E+01	0.0000E+00	0.00000
97	4.1765E+15	0.0000E+00	0.00000
98	1.0018E+02	0.0000E+00	0.00000
99	7.1175E-01	2.1205E+01	1.00000
100	3.6090E+08	0.0000E+00	0.00000
101	1.2497E+13	0.0000E+00	0.00000
102	1.4798E+11	0.0000E+00	0.00000
103	1.7462E+11	0.0000E+00	0.00000
104	1.2000E+13	0.0000E+00	0.00000
105	4.2324E+13	0.0000E+00	0.00000
106	6.9658E+12	0.0000E+00	0.00000
107	8.0770E+12	0.0000E+00	0.00000
108	2.3801E+13	-3.7776E+06	1.00000
109	3.7000E+12	0.0000E+00	0.00000
110	2.0000E+13	0.0000E+00	0.00000
111	1.0000E+13	0.0000E+00	0.00000
112	2.0000E+13	0.0000E+00	0.00000
113	8.4381E+11	0.0000E+00	0.00000
114	2.0000E+12	0.0000E+00	0.00000
115	1.1405E+13	0.0000E+00	0.00000
116	2.4070E+12	0.0000E+00	0.00000
117	8.3826E+12	0.0000E+00	0.00000
118	7.9225E+15	0.0000E+00	0.00000
119	2.2457E+14	0.0000E+00	0.00000
120	8.6958E+07	0.0000E+00	0.00000
121	3.1028E+07	0.0000E+00	0.00000
122	2.8358E+04	0.0000E+00	0.00000
123	4.0000E+12	0.0000E+00	0.00000
124	2.5566E+07	0.0000E+00	0.00000
125	2.4991E+10	7.80528E+00	1.00000
126	2.6097E+10	0.0000E+00	0.00000
127	8.6897E+11	0.0000E+00	0.00000
128	4.4875E+09	0.0000E+00	0.00000
129	9.2394E+15	0.0000E+00	0.00000
130	9.2627E+15	0.0000E+00	0.00000
131	5.0000E+12	0.0000E+00	0.00000
132	6.4495E+15	0.0000E+00	0.00000
133	3.6000E+13	0.0000E+00	0.00000
DERIVATIVES (CGS UNITS): T			
7.80578E-03 RHO			
5.34600E-08 V			
-5.05156E+00			
MIXTURE MOLECULAR WEIGHT			
28.21102			
TOTAL ENERGY EXCHANGE RATE			
(CAL-CM**3/G**2/SEC)			
5.92105E+06			
MASS FRACTION SUM			
1.00000000			
CPU TIME FOR INITIALIZATION OF LSENS =			
1.070000 S			

TABLE D.2.—Continued
(g) Continued.

TIME	2.94080E-04	SEC	AREA	1.43985E+03	SQ CM	AXIAL POSITION	4.70000E+01	CM
FLOW PROPERTIES			INTEGRATION INDICATORS					
PRESSURE	1.73125		STEPS FROM LAST PRINT	171				
VELOCITY (CM/SEC)	159765.65		AVERAGE STEP SIZE	0.41227E-01				
DENSITY (G/CM**3)	2.43084E-04		METHOD ORDER	4				
TEMPERATURE (DEG K)	2390.72							
MASS FLOW RATE (G/SEC)	5.59179E+04		TOTAL NUMBER OF STEPS	353				
ENTROPY (CAL/G/DEG K)	2.3063		FUNCT EVALUATIONS	500				
MACH NUMBER	1.6664		JACOBIAN EVALUATIONS	55				
GAMMA	1.2738							
ENTHALPY (CAL/G)	3.79465E+02							
SP. HEAT (CP) (CAL/G/DEG K)	3.35641E-01							
CHEMICAL PROPERTIES								
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR	POSITIVE DIR RATE
CH4	5.70493E-11	6.46442E-06	-5.56527E-06	1	1.8048E+09	-5.17899E-07	0.96982	0.96982
CH3	1.12286E-09	1.27235E-04	-1.13689E-04	2	1.0293E+13	4.46211E+04	0.17278	0.17278
H	4.21831E-08	4.77989E-03	-5.23517E-04	3	6.0350E+08	-7.57979E+04	0.73913	0.73913
H2	3.80956E-08	4.31672E-03	-2.31095E-04	4	1.6120E+15	7.39534E+05	0.17566	0.17566
O2	8.63035E-07	9.77931E-02	1.05168E-03	5	8.7086E+12	-5.16352E+06	0.17561	0.17561
H2O	1.73619E-10	1.96753E-05	-5.66640E-07	6	5.7333E+10	1.16355E+06	0.04321	0.04321
O	1.08967E-07	1.23473E-02	-8.59825E-04	7	6.3000E+12	8.79239E+06	0.04156	0.04156
OH	1.48973E-07	1.68806E-02	-1.31377E-04	8	6.0150E+11	1.13871E+07	1.00000	1.00000
H2O	7.22054E-07	8.18181E-02	7.44332E-04	9	1.0686E+13	-9.64762E+05	0.04718	0.04718
CH3O	6.18167E-12	7.00464E-07	-5.26294E-07	10	1.7133E+13	-5.32624E+03	0.99996	0.99996
CH2O	1.75679E-11	1.99067E-06	-1.52189E-06	11	2.1650E+13	-1.21172E+04	0.99996	0.99996
C2H6	7.07055E-14	8.01186E-09	-1.90424E-08	12	4.1470E+13	-1.56484E+05	0.99996	0.99996
C2H5	5.79157E-16	6.56260E-11	7.31591E-11	13	1.4659E+14	4.27759E+05	0.87169	0.87169
C2H4	3.29110E-13	3.72925E-08	-7.09441E-08	14	6.9815E+11	-7.50631E+01	0.98515	0.98515
CH2	1.01311E-11	1.14798E-06	-9.85971E-07	15	4.8000E+13	-1.29580E+03	0.99680	0.99680
C2H3	1.07964E-14	1.22338E-09	-2.48748E-09	16	2.0000E+13	-2.40675E+05	0.99901	0.99901
C2H2	5.82564E-14	6.60121E-09	-1.21744E-08	17	1.7525E+13	-1.01347E+04	0.99919	0.99919
HCO	1.07281E-12	1.21563E-07	-9.27399E-08	18	1.4645E+10	3.00121E+04	1.00000	1.00000
C2H2O	1.70385E-14	1.93069E-09	-2.55950E-09	19	3.7051E+12	-5.36740E+04	0.99919	0.99919
C2H	3.39526E-16	3.84728E-11	-6.59282E-11	20	1.6341E+12	-1.97671E+04	0.99195	0.99195
CO	1.31666E-07	1.49194E-02	-2.08052E-03	21	2.6014E+12	-4.23644E+04	1.00000	1.00000
C2HO	7.37796E-14	8.36019E-09	-1.44817E-08	22	8.7269E+12	-3.92109E+04	0.99996	0.99996
CH	2.12511E-12	2.40803E-07	-2.15627E-07	23	5.5630E+12	2.53274E+05	0.99841	0.99841
CO2	2.95949E-07	3.35349E-02	2.20339E-03	24	4.1950E+12	-5.25494E+04	1.00000	1.00000
H2O2	9.94278E-12	1.12665E-06	-1.63298E-07	25	6.0000E+12	-2.76687E+03	0.99996	0.99996
N2	6.47215E-06	7.33378E-01	-1.37893E-05	26	3.3000E+13	-5.32106E+04	1.00000	1.00000
HCN	3.48809E-13	3.95245E-08	-2.75224E-08	27	5.0000E+12	-1.02150E+04	0.99996	0.99996
N	1.06319E-12	1.20473E-07	1.50510E-08	28	3.0000E+13	-3.60306E+00	0.99090	0.99090
CN	2.25791E-15	2.55851E-10	-1.71466E-10	29	3.0000E+13	-1.54389E-04	0.99921	0.99921
HNCO	5.04079E-14	5.71187E-09	-1.34537E-09	30	6.9464E+06	-7.79094E+00	0.50338	0.50338
NCO	1.49924E-14	1.69884E-09	-9.46275E-10	31	1.9953E+13	-1.02390E+05	0.99909	0.99909
NH2	2.28551E-12	2.58978E-07	9.41418E-09	32	4.2420E+13	-1.04745E+05	0.99324	0.99324
NO	6.32259E-10	7.16432E-05	2.75254E-05	33	1.4435E+12	1.60360E+03	0.94988	0.94988
NH	6.76764E-14	7.66862E-09	1.26142E-09	34	3.0681E+11	-1.01478E+03	0.98752	0.98752
NO2	4.20064E-13	4.75987E-08	1.93621E-08	35	3.6462E+13	-4.88309E+03	0.86526	0.86526
N2O	6.53480E-12	7.40478E-07	1.76058E-08	36	2.0000E+13	-7.10544E+02	0.86503	0.86503
HNCO2	2.65700E-14	3.01073E-09	7.54597E-10	37	8.6261E+11	-7.62342E+04	1.00000	1.00000
HNCO3	3.10331E-18	3.51645E-13	9.60823E-14	38	1.2020E+12	-6.1248E+04	1.00000	1.00000
HNO	8.99356E-14	1.01909E-08	1.93850E-09	39	1.0000E+13	5.02556E+04	1.00000	1.00000
				40	5.0000E+13	-5.62043E+04	0.86517	0.86517
				41	3.0000E+13	-3.60992E+01	0.99998	0.99998
				42	6.5640E+12	-2.43154E+00	0.99994	0.99994
				43	1.0000E+13	-6.96815E-02	1.00000	1.00000
				44	2.8000E+13	-1.83031E+04	0.99986	0.99986
				45	3.9885E+12	-1.35077E+03	0.45802	0.45802
				46	5.4917E+12	3.40106E+04	0.94055	0.94055
				47	1.3923E+13	1.70244E+02	0.45629	0.45629
				48	9.2820E+12	-4.49845E+01	0.45818	0.45818
				49	2.0000E+13	-6.42681E+04	1.00000	1.00000
				50	6.5476E+10	-2.49452E+04	0.65940	0.65940
				51	5.0000E+13	-2.28976E+03	0.99874	0.99874
				52	2.2108E+12	-6.20734E+06	1.00000	1.00000
				53	2.0000E+13	-7.38735E+06	1.00000	1.00000
				54	1.9692E+09	4.62373E+05	0.99209	0.99209
				55	2.3304E+13	-2.99380E+07	0.99980	0.99980
				56	1.0794E+13	-1.89509E+06	0.99980	0.99980
				57	1.6719E+13	-6.57142E+06	0.99980	0.99980
				58	1.3828E+11	-6.74653E+02	0.99976	0.99976
				59	1.4669E+13	-2.66371E+04	0.99489	0.99489
				60	2.0000E+13	-1.15848E+06	0.79425	0.79425
				61	8.2479E+07	1.25085E+06	0.82486	0.82486
				62	2.2161E+11	9.59954E+05	0.99563	0.99563
				63	1.6856E+11	2.53483E+06	0.99564	0.99564
				64	2.2161E+11	-5.98533E+06	0.99564	0.99564
				65	3.7000E+12	-2.51915E+06	1.00000	1.00000
				66	1.0000E+13	-2.23620E+07	1.00000	1.00000
				67	5.6491E+12	-5.05691E+07	0.99999	0.99999
				68	2.0299E+11	-2.06745E+03	0.93050	0.93050
				69	7.0612E+12	-2.93049E+06	0.93048	0.93048
				70	2.6049E+13	-4.29786E+05	0.93026	0.93026
				71	5.0000E+12	-6.11830E+02	0.99982	0.99982
				72	4.0000E+13	-9.06783E+03	1.00000	1.00000
				73	3.0000E+13	-1.67365E+07	0.98041	0.98041
				74	3.0000E+13	-5.14479E+06	0.99579	0.99579
				75	3.0000E+13	-8.39724E+06	0.99579	0.99579
				76	2.0000E+13	-1.35621E+06	0.99577	0.99577
				77	1.0941E+13	2.22615E+07	0.83069	0.83069
				78	1.0125E+15	-2.71219E+08	0.98288	0.98288

TABLE D.2.—Continued.
(g) Concluded

79	1.0922E+08	-5.31228E+05	0.31308
80	3.3785E+11	-8.69108E+08	0.31190
81	4.6079E+11	-8.93559E+06	0.85228
82	1.4245E+12	9.41893E+06	0.00029
83	5.9875E+12	1.06652E+08	0.00172
84	2.3242E+13	1.05930E+07	0.00348
85	4.6535E+13	-2.37923E+08	0.78420
86	4.0509E+13	-5.16523E+08	0.78495
87	8.0000E+12	-1.85830E+08	0.78489
88	1.0698E+14	-3.53684E+08	0.78532
89	4.1000E+11	-6.47435E+06	0.88118
90	4.5145E+12	-3.39511E+06	0.88156
91	1.8000E+12	2.51669E+04	0.44940
92	7.8000E+11	-3.66899E+05	0.97457
93	9.9547E+12	-2.27140E+07	0.02108
94	1.3132E+13	-6.02479E+07	0.00318
95	1.8021E+15	-1.39117E+09	0.88429
96	3.1804E+05	-4.93960E+08	0.97511
97	2.9698E+15	-2.03454E+08	0.97512
98	3.6856E+05	-2.55127E+07	0.97503
99	1.2242E+04	-7.35218E+06	0.97507
100	1.8327E+09	1.39732E+03	1.00000
101	1.9663E+13	5.61948E+03	0.90925
102	7.9177E+11	9.94238E+03	0.90956
103	2.2187E+11	-2.54811E+03	0.94536
104	1.2000E+13	-3.84606E+03	0.99974
105	7.0704E+13	-5.08990E+03	0.54712
106	1.5040E+13	4.93186E+02	0.24782
107	1.6710E+13	-1.40358E+03	0.26496
108	2.5926E+13	-2.97245E+03	0.54790
109	3.7000E+12	2.47856E+01	0.54184
110	2.0000E+13	-5.65425E+04	0.99999
111	1.0009E+13	-4.75669E-01	0.99306
112	2.0000E+13	-7.62101E+03	0.99937
113	1.9745E+12	-1.81552E+03	1.00000
114	2.0000E+12	-3.27179E+03	0.99980
115	1.6047E+13	-6.76546E+03	0.07033
116	2.3107E+12	-1.92250E+02	0.00929
117	8.8210E+12	-2.45625E+05	0.78294
118	7.1743E+15	-4.78280E+06	0.88517
119	2.5465E+14	-1.74329E+06	0.78331
120	6.4816E+09	-6.95800E+06	0.98006
121	1.5012E+09	-2.72471E+06	0.98010
122	1.9267E+07	1.72713E+07	0.99832
123	4.0000E+12	-2.33353E+00	0.99568
124	2.8298E+09	-7.22372E+05	0.86721
125	2.7449E+11	-2.12419E+05	0.81230
126	2.5451E+11	-1.08668E+05	0.99999
127	3.1613E+12	-7.46464E+05	0.81262
128	5.3598E+10	-2.80283E+03	0.88464
129	6.6758E+15	-8.04826E-02	0.00003
130	8.0093E+15	-6.18944E+03	0.00110
131	5.0000E+12	-1.68918E+04	0.96240
132	6.1269E+15	-4.06066E+05	0.33593
133	3.6000E+13	-5.47495E+05	0.96252

DERIVATIVES (CGS UNITS): T 2.13842E+01 RHO -1.82919E-06 V 1.22400E+00
MIXTURE MOLECULAR WEIGHT 27.54458 TOTAL ENERGY EXCHANGE RATE -4.71024E+09 MASS FRACTION SUM 1.00000003
(CAL-CM**3/GMM2/SEC)

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 1.128000E+01 S UP TO THIS TIME - 2.184000E+01 S

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS - 353
TOTAL NO. OF DERIVATIVE EVALUATIONS - 500
TOTAL NO. OF JACOBIAN EVALUATIONS - 55
TOTAL CPU TIME - 21.840000 S

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 24.139996 S

(LSENS) READ DATA FOR NEXT CASE

(h) Case 8

CC 123456789012345678901234567890123456789012345678901234567890123456789012345678901234567890

DISTANCE-AREA VERSION LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM NASA LEWIS RESEARCH CENTER

ISENS METHANE - AIR WITH AREA AND TEMPERATURE PROFILES OF CASE 6 CASE 8

REACTION NUMBER	REACTION				REACTION RATE VARIABLES		ACTIVATION ENERGY			
					A	H				
1	M	+	1*CH4	=	1*CH3	+	1*H	2.00000E+17	0.0000	88000.00
2	1*H	+	1*CH4	=	1*CH3	+	1*H2	1.26000E+14	0.0000	11900.00
3	1*CH4	+	1*O2	=	1*CH3	+	1*HO2	7.94000E+13	0.0000	56000.00
4	1*O	+	1*CH4	=	1*CH3	+	1*OH	1.90000E+14	0.0000	11720.00
5	1*OH	+	1*CH4	=	1*CH3	+	1*H2O	2.50000E+13	0.0000	5010.00
6	1*CH3	+	1*O2	=	1*CH3O	+	1*O	2.40000E+13	0.0000	28680.00
7	1*CH3	+	1*OH	=	1*CH3O	+	1*H	6.30000E+12	0.0000	0.00
8	M	+	1*CH3O	=	1*CH2O	+	1*H	5.00000E+13	0.0000	21000.00
9			2*CH3	=	1*CH2H	+		2.40000E+14	0.0000	0.00
10	1*H	+	1*CH2H	=	1*CH2H5	+	1*H2	1.32000E+14	0.0000	9700.00
11	1*O	+	1*CH2H6	=	1*CH2H5	+	1*OH	1.13000E+14	0.0000	7850.00
12	1*OH	+	1*CH2H6	=	1*CH2H5	+	1*H2O	8.70000E+13	0.0000	3520.00
13	M	+	1*CH2H5	=	1*CH2H4	+	1*H	1.00000E+17	0.0000	31000.00
14	1*CH2H5	+	1*O2	=	1*CH2H4	+	1*HO2	2.00000E+12	0.0000	5000.00
15	1*H	+	1*CH2H5	=	1*CH2H4	+	1*H2	4.80000E+13	0.0000	0.00
16	1*CH3	+	1*CH2	=	1*CH2H4	+	1*H	2.00000E+13	0.0000	0.00
17	1*H	+	1*CH2H4	=	1*H2	+	1*CH2H3	1.50000E+14	0.0000	10200.00
18	M	+	1*CH2H4	=	1*CH2H2	+	1*H2	2.60000E+17	0.0000	79300.00
19	1*CH2H4	+	1*OH	=	1*CH2H3	+	1*H2O	4.80000E+12	0.0000	1230.00
20	1*CH2H4	+	1*OH	=	1*CH3	+	1*CH2O	2.00000E+12	0.0000	960.00
21	1*CH2H4	+	1*O	=	1*CH3	+	1*HCO	3.30000E+12	0.0000	1130.00
22	1*CH2H4	+	1*O	=	1*CH2O	+	1*CH2	2.50000E+13	0.0000	5000.00
23	M	+	1*CH2H3	=	1*CH2H2	+	1*H	3.00000E+15	0.0000	32000.00
24	1*CH2H3	+	1*O2	=	1*CH2O	+	1*HCO	3.98000E+12	0.0000	-250.00
25	1*CH2H3	+	1*H	=	1*CH2H2	+	1*H2	6.00000E+12	0.0000	0.00
26	1*CH2H3	+	1*O	=	1*CH2H2O	+	1*H	3.30000E+13	0.0000	0.00
27	1*CH2H3	+	1*OH	=	1*CH2H2	+	1*H2O	5.00000E+12	0.0000	0.00
28	1*CH2H3	+	1*CH2	=	1*CH2H2	+	1*CH3	3.00000E+13	0.0000	0.00
29	1*CH2H3	+	1*CH2H	=	2*CH2H2	+		3.00000E+13	0.0000	0.00
30	M	+	1*CH2H2	=	1*CH2H	+	1*H	4.20000E+16	0.0000	107000.00
31	1*CH2H2	+	1*O	=	1*CH2	+	1*CO	1.60000E+14	0.0000	9890.00
32	1*CH2H2	+	1*O	=	1*C2HO	+	1*H	4.00000E+14	0.0000	10660.00
33	1*CH2H2	+	1*OH	=	1*CH2H	+	1*H2O	6.30000E+12	0.0000	7000.00
34	1*CH2H2	+	1*OH	=	1*CH2H2O	+	1*H	3.20000E+11	0.0000	200.00
35	1*CH2H	+	1*O2	=	1*CH2HO	+	1*O	5.00000E+13	0.0000	1500.00
36	1*CH2H	+	1*OH	=	1*CH2HO	+	1*H	2.00000E+13	0.0000	0.00
37	1*CH2HO	+	1*O2	=	2*CO	+	1*OH	1.46000E+12	0.0000	2500.00
38	1*CH2HO	+	1*O	=	2*CO	+	1*H	1.20000E+12	0.0000	0.00
39	1*CH2HO	+	1*OH	=	2*HCO	+		1.00000E+13	0.0000	0.00
40	1*CH2HO	+	1*H	=	1*CH2	+	1*CO	5.00000E+13	0.0000	0.00
41	1*CH2HO	+	1*CH2	=	1*CH2H3	+	1*CO	3.00000E+13	0.0000	0.00
42	1*CH2HO	+	1*CH2	=	1*CH2O	+	1*CH2H	1.00000E+13	0.0000	2000.00
43			2*CH2HO	=	1*CH2H2	+	2*CO	1.00000E+13	0.0000	0.00
44	1*CH2H2O	+	1*OH	=	1*CH2O	+	1*HCO	2.80000E+13	0.0000	0.00
45	1*CH2HO	+	1*OH	=	1*CH2HO	+	1*H2O	7.50000E+12	0.0000	3000.00
46	1*CH2HO	+	1*H	=	1*CH3	+	1*CO	1.13000E+13	0.0000	3428.00
47	1*CH2HO	+	1*H	=	1*CH2HO	+	1*H2	7.50000E+13	0.0000	8000.00
48	1*CH2HO	+	1*O	=	1*CH2HO	+	1*OH	5.00000E+13	0.0000	8000.00
49	1*CH2HO	+	1*O	=	1*CH2O	+	1*CO	2.00000E+13	0.0000	0.00
50	M	+	1*CH2H2O	=	1*CH2	+	1*CH	2.00000E+16	0.0000	6000.00
51	1*CH2H	+	1*O	=	1*CO	+	1*CH	5.00000E+13	0.0000	0.00
52	1*CH3O	+	1*O2	=	1*CH2O	+	1*HO2	1.00000E+13	0.0000	7170.00
53	1*CH3O	+	1*H	=	1*CH2O	+	1*H2	2.00000E+13	0.0000	0.00
54	M	+	1*CH2O	=	1*HCO	+	1*H	5.00000E+16	0.0000	81000.00
55	1*CH2O	+	1*OH	=	1*HCO	+	1*H2O	3.00000E+13	0.0000	1200.00
56	1*CH2O	+	1*H	=	1*HCO	+	1*H2	2.50000E+13	0.0000	3990.00
57	1*CH2O	+	1*O	=	1*HCO	+	1*OH	3.50000E+13	0.0000	3510.00
58	1*CH3	+	1*CH2O	=	1*CH4	+	1*HCO	1.00000E+10	0.5000	6000.00
59	1*CH3	+	1*HCO	=	1*CH4	+	1*CO	3.00000E+11	0.5000	0.00
60	1*CH3	+	1*HO2	=	1*CH3O	+	1*OH	2.00000E+13	0.0000	0.00
61	M	+	1*CH3	=	1*CH2	+	1*H	1.95000E+16	0.0000	91600.00
62	1*H	+	1*CH3	=	1*H2	+	1*CH2	2.70000E+11	0.6700	2570.00
63	1*O	+	1*CH3	=	1*OH	+	1*CH2	1.90000E+11	0.6800	2570.00
64	1*OH	+	1*CH3	=	1*H2O	+	1*CH2	2.70000E+11	0.6700	2570.00
65	1*CH	+	1*CO2	=	1*HCO	+	1*CO	3.70000E+12	0.0000	0.00
66	1*CH	+	1*O2	=	1*HCO	+	1*O	1.00000E+13	0.0000	0.00
67	1*CH2	+	1*O2	=	1*CH2O	+	1*O	5.00000E+11	0.5000	6960.00
68	1*CH2	+	1*O	=	1*CH	+	1*OH	2.00000E+11	0.7000	2580.00
69	1*CH2	+	1*OH	=	1*CH	+	1*H2O	5.00000E+11	0.5000	5900.00
70	1*CH2	+	1*H	=	1*CH	+	1*H2	3.20000E+11	0.7000	4970.00
71			2*CH2	=	1*CH2H5	+	1*H	5.00000E+12	0.0000	0.00
72			2*CH2	=	1*CH2H2	+	1*H2	2.00000E+13	0.0000	0.00
73	1*HCO	+	1*O2	=	1*CO	+	1*HO2	3.00000E+13	0.0000	0.00
74	1*HCO	+	1*O	=	1*CO	+	1*OH	3.00000E+13	0.0000	0.00
75	1*HCO	+	1*OH	=	1*CO	+	1*H2O	3.00000E+13	0.0000	0.00
76	1*HCO	+	1*H	=	1*CO	+	1*H2	2.00000E+13	0.0000	0.00

TABLE D.2.—Continued.

(h) Continued.

77	M	+	1*HC0	=	1*H	+	1*CO	2.90000E+14	0.0000	15570.00
78	1*CO	+	1*O	=	1*CO2	+	M	2.40000E+15	0.0000	4100.00
79	1*CO	+	1*O2	=	1*CO2	+	1*O	2.50000E+12	0.0000	47490.00
80	1*CO	+	1*OH	=	1*CO2	+	1*H	4.17000E+11	0.0000	1000.00
81	1*CO	+	1*H2O	=	1*CO2	+	1*OH	5.75000E+13	0.0000	22930.00
82	1*O	+	1*H2O	=	2*OH			6.80000E+13	0.0000	18365.00
83	1*H	+	1*O2	=	1*OH	+	1*O	1.89000E+14	0.0000	16400.00
84	1*H	+	1*H2	=	1*OH	+	1*H	4.20000E+14	0.0000	13750.00
85	1*H	+	1*H2O	=	1*H2	+	1*O2	7.28000E+13	0.0000	2126.00
86	1*O	+	1*H2O	=	1*OH	+	1*O2	5.00000E+13	0.0000	1000.00
87	1*H2O	+	1*OH	=	1*H2O	+	1*O2	8.00000E+12	0.0000	0.00
88	1*H	+	1*H2O	=	2*OH			1.34000E+14	0.0000	1070.00
89	1*H2	+	1*H2O	=	1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00
90	1*OH	+	1*H2O2	=	1*H2O	+	1*H2O2	6.10000E+12	0.0000	1430.00
91			2*H2O	=	1*H2O2	+	1*O2	1.80000E+12	0.0000	0.00
92	1*H	+	1*H2O2	=	1*OH	+	1*H2O	7.80000E+11	0.0000	0.00
93	M	+	1*H2O2	=	2*OH			1.44000E+17	0.0000	45510.00
94	1*H2	+	1*OH	=	1*H2O	+	1*H	4.74000E+13	0.0000	6098.00
95	1*H	+	1*O2	=	1*H2O	+	M	1.46000E+15	0.0000	-1000.00
96	M	+	1*H2O	=	1*H	+	1*OH	1.30000E+15	0.0000	105140.00
97	1*H	+	1*O	=	1*OH	+	M	7.10000E+18	-1.0000	0.00
98	M	+	1*H2	=	2*H			2.20000E+14	0.0000	96000.00
99	M	+	1*O2	=	2*O			1.80000E+18	-1.0000	118020.00
100	1*CH	+	1*H2	=	1*HCN	+	1*H	1.00000E+11	0.0000	19000.00
101	1*CN	+	1*H2	=	1*HCN	+	1*H	6.00000E+13	0.0000	5300.00
102	1*O	+	1*HCN	=	1*OH	+	1*CN	1.40000E+11	0.6800	16900.00
103	1*OH	+	1*HCN	=	1*HHCN	+	1*H	4.00000E+11	0.0000	2800.00
104	1*CN	+	1*O	=	1*CO	+	1*H	1.20000E+13	0.0000	0.00
105	1*CN	+	1*OH	=	1*HCO	+	1*H	2.50000E+14	0.0000	6000.00
106	1*H2	+	1*HCO	=	1*HHCN	+	1*H	1.00000E+14	0.0000	9000.00
107	1*HHCN	+	1*H	=	1*H2	+	1*CO	1.00000E+14	0.0000	8500.00
108	1*CN	+	1*O2	=	1*HCO	+	1*O	3.20000E+13	0.0000	1000.00
109	1*CN	+	1*CO2	=	1*HCO	+	1*CO	3.70000E+12	0.0000	0.00
110	1*O	+	1*HCO	=	1*H2	+	1*CO	2.00000E+13	0.0000	0.00
111	1*H	+	1*HCO	=	1*H2	+	1*CO	1.00000E+13	0.0000	0.00
112	1*H	+	1*HCO	=	1*H2	+	1*CO	2.00000E+13	0.0000	0.00
113	1*CH	+	1*H2	=	1*H	+	1*HCO	1.60000E+13	0.0000	9940.00
114	1*CH	+	1*H2	=	1*O	+	1*HCO	2.00000E+12	0.0000	0.00
115	1*H	+	1*H2	=	1*H	+	1*H2O	5.00000E+11	0.5000	2000.00
116	1*H2O	+	1*H2	=	1*H2O	+	1*OH	2.09000E+12	0.0000	-477.00
117	1*O	+	1*H2O	=	1*H2	+	1*O2	1.00000E+13	0.0000	596.00
118	1*H2O	+	1*O	=	1*H2O	+	M	5.62000E+15	0.0000	-1160.00
119	1*H2O2	+	1*H	=	1*H2O	+	1*OH	3.47000E+14	0.0000	110.00
120	1*H2O	+	1*H	=	1*H	+	1*OH	2.63000E+14	0.0000	50410.00
121	1*H2O	+	1*O	=	1*H	+	1*O2	3.80000E+09	1.0000	41370.00
122	1*O	+	1*H2	=	1*H2O	+	1*H	1.80000E+14	0.0000	76250.00
123	1*H	+	1*H2O	=	2*H2O			4.00000E+12	0.0000	0.00
124	M	+	1*H2O	=	1*H2	+	1*O	6.92000E+23	-2.5000	65000.00
125	1*O	+	1*H2O	=	1*H2	+	1*O2	1.00000E+14	0.0000	28020.00
126	1*O	+	1*H2O	=	2*H2O			6.92000E+13	0.0000	26630.00
127	1*H2O	+	1*H	=	1*H2	+	1*OH	7.59000E+13	0.0000	15100.00
128	1*H2O2	+	1*H2	=	1*H2O2	+	1*H	2.40000E+13	0.0000	29000.00
129	1*OH	+	1*H2O	=	1*H2O2	+	M	3.00000E+15	0.0000	-3800.00
130	1*OH	+	1*H2O	=	1*H2O2	+	M	5.60000E+15	0.0000	-1700.00
131	1*H2O	+	1*H	=	1*H2	+	1*H2O	5.00000E+12	0.0000	0.00
132	1*H	+	1*H2O	=	1*H2O	+	M	5.40000E+15	0.0000	-600.00
133	1*H2O	+	1*OH	=	1*H2O	+	1*H2O	3.60000E+13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	, 93) =	2.30000	M(O2	, 93) =	0.78000	M(H2O	, 93) =	6.00000	M(H2O2	, 93) =	6.60000
M(O2	, 95) =	1.30000	M(H2	, 95) =	1.30000	M(H2O	, 95) =	21.30000	M(CO2	, 95) =	7.00000
M(H2	, 96) =	4.00000	M(O2	, 96) =	1.50000	M(H2O	, 96) =	20.00000	M(H2	, 96) =	1.50000
M(CO2	, 96) =	4.00000	M(H2	, 98) =	4.10000	M(O2	, 98) =	2.00000	M(H2O	, 98) =	15.00000
M(H2	, 98) =	2.00000	M(O2	, 129) =	0.70000	M(H2	, 129) =	1.40000			

TIME 1.87696E-04 SEC

AREA 1.02322E+03 SQ CM

AXIAL POSITION 3.00000E+01 CM

FLOW PROPERTIES

PRESSURE	1.73000
(ATM)	
VELOCITY	159827.59
(CM/SEC)	
DENSITY	3.41933E-04
(G/CM**3)	
TEMPERATURE	1738.22
(DEG K)	
MASS FLOW RATE	5.59193E+04
(G/SEC)	
ENTROPY	2.1560
(CAL/G/DEG K)	
MACH NUMBER	1.9774
GAMMA	1.2743
ENTHALPY	3.79343E+02
(CAL/G)	
SP. HEAT (CP)	3.27469E-01
(CAL/G/DEG K)	

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	80
AVERAGE STEP SIZE	0.38091E+00
METHOD ORDER	5
TOTAL NUMBER OF STEPS	80
FUNCT EVALUATIONS	103
JACOBIAN EVALUATIONS	17

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST COS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/CM**2/SEC)	NET RATE/POSITIVE DIR RATE
CH4	4.91663E-07	4.05355E-02	-2.04428E-03	1	1.7243E+06	4.22765E+06	0.45858
CH3	1.87424E-08	1.54523E-03	2.41396E-04	2	4.0194E+12	8.59979E+05	0.85780
H	1.00305E-10	8.26970E-06	2.62788E-06	3	7.2249E+06	-4.50456E+06	0.54351
H2	8.70599E-09	7.1771E-04	1.82136E-04	4	6.3852E+12	-1.07993E+07	0.99612
O2	2.33987E-06	1.92912E-01	-1.51872E-03	5	5.8617E+12	-1.74675E+08	0.08245
H2O	2.14976E-09	1.77238E-04	1.86213E-05	6	5.9459E+09	6.31448E+07	0.98890
O	1.62638E-10	1.34088E-05	3.58719E-06	7	6.3000E+12	-1.90904E+07	0.76078
OH	5.01110E-10	4.13143E-05	1.7881E-05	8	1.1445E+11	4.90885E+07	1.00000
H2O	9.19391E-08	7.57998E-03	2.06236E-03	9	1.2139E+13	-3.56356E+08	0.10895
CH3O	2.01636E-10	1.66240E-05	3.28997E-06	10	7.9611E+12	-6.25094E+05	0.99997

TABLE D.2.—Continued

(h) Continued.

CH20	3.40861E-08	2.81025E-03	3.90598E-04	11	1.1643E+13	-1.03316E+06	1.00000
C2H6	1.48603E-08	1.22517E-03	1.90737E-04	12	3.1401E+13	-4.23370E+07	1.00000
C2H5	1.84233E-12	1.51892E-07	-1.11263E-08	13	1.2656E+13	9.00755E+07	0.96218
C2H4	6.93688E-09	5.71916E-04	2.45640E-04	14	4.7029E+11	-1.89483E+05	0.84696
CH2	1.02897E-12	8.48343E-08	5.54917E-08	15	4.8000E+13	-4.92020E+03	0.99007
C2H3	1.26767E-12	1.04514E-07	6.77191E-08	16	2.0000E+13	-2.06356E+05	0.99973
C2H2	1.13146E-10	9.32836E-06	6.13771E-06	17	7.8275E+12	-1.14722E+05	0.99970
HCO	4.78502E-12	3.94504E-07	1.77276E-07	18	2.7825E+07	8.34820E+05	1.00000
C2H2O	6.17333E-13	5.08965E-08	3.52493E-08	19	3.3619E+12	-1.74650E+06	0.99996
C2H	6.19563E-16	5.10803E-11	-2.48645E-11	20	1.5147E+12	2.44946E+04	0.03569
CO	1.45973E-08	1.20348E-03	5.18771E-04	21	2.3792E+12	-6.16035E+05	1.00000
C2HO	2.20257E-13	1.81592E-08	1.64241E-08	22	5.8787E+12	-4.19932E+05	0.99990
CH	1.45162E-16	1.19680E-11	5.61504E-12	23	2.8425E+11	1.64693E+06	0.99779
CO2	9.07745E-11	7.48396E-06	4.75308E-06	24	4.2787E+12	-8.62319E+06	1.00000
H2O2	2.85151E-12	2.35095E-07	3.47544E-08	25	6.0000E+12	-3.91618E+02	0.99942
N2	9.10447E-06	7.50624E-01	-8.48242E-10	26	3.3000E+13	-4.71286E+03	1.00000
HCN	4.05268E-16	3.34126E-11	1.22506E-11	27	5.0000E+12	-2.03896E+03	0.99993
N	5.18291E-17	4.27309E-12	1.22165E-12	28	3.0000E+13	-1.82891E+01	0.83495
CN	1.64557E-17	1.35670E-12	1.35672E-15	29	3.0000E+13	-1.63287E-02	0.97593
HNCO	1.01663E-12	8.38170E-08	2.70655E-09	30	1.4789E+03	2.00478E+00	0.90810
NC0	5.76588E-14	4.75372E-09	-3.88585E-09	31	9.1334E+12	-6.87260E+04	1.00000
NH2	2.62917E-14	2.16764E-09	8.64340E-10	32	1.8271E+13	-6.6547E+04	1.00000
NO	7.73732E-14	6.37908E-09	4.33469E-10	33	8.3027E+11	3.19646E+03	0.99702
NH	2.87343E-14	2.36902E-09	-5.25303E-11	34	3.0200E+11	-3.33966E+03	0.99997
NO2	1.04519E-14	8.61711E-10	5.99231E-11	35	3.2387E+13	-1.25336E+04	0.99999
N2O	4.01764E-14	3.31237E-09	7.78525E-10	36	2.0000E+13	-2.53959E+00	0.99655
HNO2	4.10931E-19	3.38795E-14	9.28872E-15	37	7.0798E+11	-2.55945E+05	1.00000
HNO3	7.84827E-21	6.47056E-16	1.84475E-16	38	1.2020E+12	-3.63790E+01	1.00000
HNO	1.53856E-18	1.26848E-13	3.57553E-14	39	1.0000E+13	-2.55052E+02	0.99999
				40	5.0000E+13	-2.27145E+02	0.97460
				41	3.0000E+13	-5.53197E+00	1.00000
				42	5.6045E+12	-2.92364E-01	0.91892
				43	1.0000E+13	-3.15858E-01	1.00000
				44	2.8000E+13	1.58583E+03	0.58445
				45	3.1468E+12	-9.65093E+01	0.67340
				46	4.1886E+12	1.29688E+03	0.94764
				47	7.3996E+12	1.42157E+01	0.62214
				48	4.9330E+12	-1.32298E+00	0.92770
				49	2.0000E+13	-1.75647E+03	1.00000
				50	5.7163E+08	2.10655E+03	0.74408
				51	5.0000E+13	-3.15580E+00	1.00000
				52	1.2546E+12	-1.57440E+08	1.00000
				53	2.0000E+13	-2.89578E+05	1.00000
				54	3.2710E+06	1.04331E+06	0.99995
				55	2.1195E+13	-8.98342E+07	1.00000
				56	7.8753E+12	-3.22448E+06	0.99999
				57	1.2669E+13	-7.28970E+06	1.00000
				58	7.3394E+10	-5.86167E+06	0.99991
				59	1.2508E+13	-8.58946E+05	0.99995
				60	2.0000E+13	-1.52351E+08	0.99998
				61	5.9291E+04	1.24694E+04	0.98660
				62	2.3692E+10	2.04299E+03	0.99648
				63	1.7812E+10	5.38694E+03	0.99990
				64	2.3492E+10	-1.80751E+04	0.99957
				65	3.7000E+12	-2.65679E-02	0.99599
				66	1.0000E+13	-2.09304E+03	1.00000
				67	2.7793E+12	-3.46240E+06	1.00000
				68	2.1146E+10	-1.77309E-02	0.99991
				69	3.7775E+12	-2.90787E+02	0.99957
				70	1.4071E+13	-3.03568E+01	0.99654
				71	5.0000E+12	-3.19027E+00	0.99998
				72	4.0000E+13	-4.72748E+01	1.00000
				73	3.0000E+13	-1.04318E+08	0.99988
				74	3.0000E+13	-1.73829E+04	1.00000
				75	3.0000E+13	-6.39424E+04	1.00000
				76	2.0000E+13	-7.30031E+03	0.99999
				77	3.1971E+12	2.42608E+07	0.99997
				78	7.3234E+14	-2.29399E+04	1.00000
				79	2.5222E+06	-5.95223E+03	1.00000
				80	3.1218E+11	-4.85167E+05	0.99974
				81	7.5272E+11	-1.18821E+06	1.00000
				82	3.3377E+11	5.60904E+05	0.78662
				83	1.6385E+12	1.50100E+07	0.99735
				84	7.8421E+12	1.72419E+05	0.97268
				85	3.9339E+13	-3.56870E+06	0.93509
				86	3.7432E+13	-5.66904E+06	0.99823
				87	8.0000E+12	-4.94382E+06	0.99199
				88	9.8304E+13	-6.15819E+06	1.00000
				89	5.6869E+10	1.71386E+05	0.98969
				90	4.0321E+12	1.84062E+04	0.91649
				91	1.8000E+12	-2.38757E+06	0.99933
				92	7.8000E+11	-1.29745E+02	0.99994
				93	2.7309E+11	4.11537E+06	0.99826
				94	8.1108E+12	-3.98209E+06	0.87659
				95	1.9502E+15	1.07256E+07	0.75285
				96	7.8431E+01	-4.30735E+03	0.96759
				97	4.0846E+15	-7.02361E+02	0.99282
				98	1.8714E+02	-1.01453E+02	0.73735
				99	1.5007E+00	2.73343E+01	0.63000
100					4.0841E+08	1.51216E-02	1.00000
101					1.2935E+13	-3.09113E-01	0.99521
102					1.6770E+11	-9.53688E-03	0.82456
103					1.7783E+11	1.15967E+00	0.99633
104					1.2000E+13	-2.11495E-02	1.00000
105					4.4010E+13	2.66821E+00	0.97381
106					7.3861E+12	-3.15352E+02	0.96577
107					8.5365E+12	-6.51284E+01	0.99293
108					2.3956E+13	-4.49856E+01	0.89861
109					3.7000E+12	-1.21137E+01	0.99999
110					2.0000E+13	-1.64033E+02	1.00000
111					1.0000E+13	-4.53663E-05	1.00000
112					2.0000E+13	-3.52399E+01	0.99986
113					9.0021E+11	-3.49269E-06	0.99876
114					2.0000E+12	-1.38230E-05	0.99984
115					1.1683E+13	-5.05361E+01	0.99975
116					2.3995E+12	-1.58091E+01	0.96025
117					8.4152E+12	-5.36672E+00	0.95539
118					7.8629E+15	4.47638E+01	0.98349
119					2.2673E+14	-5.92424E+01	0.99988
120					1.2073E+08	-4.63221E-01	0.99916
121					4.1530E+07	-6.36365E+01	1.00000
122					4.6581E+04	4.43828E+01	1.00000
123					4.0000E+12	-1.43670E-06	1.00000

TABLE D.2.—Continued.

(h) Continued.

		124	3.6920E+07	-2.59910E+02	0.97684
		125	2.9991E+10	1.53282E+01	0.99143
		126	3.1036E+10	-6.14560E-02	1.00000
		127	9.5871E+11	-1.42067E+00	0.69023
		128	5.4198E+09	1.06138E-01	0.99950
		129	9.0137E+15	-7.80955E-05	0.00034
		130	9.1608E+15	2.06336E-01	0.10093
		131	5.0000E+12	-2.55037E-04	0.70678
		132	6.4244E+15	-2.67106E-02	0.10426
		133	3.6000E+13	-1.59443E-02	0.96381

DERIVATIVES (CGS UNITS): T	5.52418E+00	RHO	-1.17628E-06	V	3.11322E+00
MIXTURE MOLECULAR WEIGHT	28.19088	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	-8.47574E+08	MASS FRACTION SUM	1.00000000

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 4.559998E+00 5 UP TO THIS TIME - 4.559998E+00 5

TIME 2.94056E-04 SEC AREA 1.43983E+03 SQ CM AXIAL POSITION 4.70000E+01 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.73099
VELOCITY (CM/SEC)	159772.69
DENSITY (G/CM**3)	2.43059E-04
TEMPERATURE (DEG K)	2389.90
MASS FLOW RATE (G/SEC)	5.59145E+04
ENTROPY (CAL/G/DEG K)	2.3067
MACH NUMBER	1.6664
GAMMA	1.2739
ENTHALPY (CAL/G)	3.80606E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.35629E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	88
AVERAGE STEP SIZE	0.80410E-01
METHOD ORDER	3
TOTAL NUMBER OF STEPS	201
FUNCT EVALUATIONS	329
JACOBIAN EVALUATIONS	42

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	NET RATE/POSI- TIVE DIR RATE
CH4	6.02064E-11	6.82084E-06	-5.87364E-06	1	1.7934E+09	-5.63144E+07	0.97085
CH3	1.19228E-09	1.35075E-04	-1.20699E-04	2	1.0284E+13	4.87310E+04	0.17515
H	4.30898E-08	4.88168E-03	-5.41198E-04	3	6.0084E+08	-8.10028E+04	0.74230
H2	3.85719E-08	4.36984E-03	-2.36473E-04	4	1.6106E+13	8.02175E+05	0.17803
O2	8.63190E-07	9.77915E-02	-1.07343E-03	5	8.7054E+12	-3.40203E+06	0.17782
H2O	1.74059E-10	1.97193E-05	-5.79197E-07	6	5.7214E+10	1.20753E+06	0.04232
O	1.10579E-07	1.25275E-02	-8.86814E-04	7	6.3000E+12	9.19504E+06	0.04069
OH	1.49823E-07	1.69736E-02	-1.37747E-04	8	6.0059E+11	1.18884E+07	1.00000
H2O	7.20497E-07	8.16257E-02	7.73146E-04	9	1.0687E+13	-1.07608E+06	0.04666
CH3O	6.46103E-12	7.31976E-07	-5.46729E-07	10	1.7121E+13	-6.17155E+03	0.99996
CH2O	1.83927E-11	2.08375E-06	-1.59315E-06	11	4.1466E+13	-1.39501E+04	0.99996
C2H6	3.02425E-14	9.09074E-09	-4.07503E-08	12	1.4626E+14	-1.78596E+05	0.99996
C2H5	6.65571E-16	7.54031E-11	-7.03961E-10	13	1.4626E+14	4.90362E+05	0.87112
C2H4	3.70903E-13	4.20199E-08	-7.96112E-08	14	6.9790E+11	-8.62886E+01	0.98542
CH2	1.08162E-11	1.22538E-06	-1.05343E-06	15	4.8000E+13	-1.52163E+03	0.99690
C2H3	1.23486E-14	1.39899E-09	-3.10263E-09	16	2.0000E+13	-2.72888E+05	0.99900
C2H2	6.54397E-14	7.41372E-09	-1.35717E-08	17	1.7512E+13	-1.16610E+04	0.99919
HCO	1.13443E-12	1.28520E-07	-9.92805E-08	18	1.4561E+10	3.36432E+04	1.00000
C2H2O	1.85990E-14	2.10709E-09	-2.84900E-09	19	3.7048E+12	-6.08421E+04	0.99919
C2H	3.82673E-16	4.33536E-11	-7.74788E-11	20	1.6340E+12	-2.24112E+04	0.99211
CO	1.33005E-07	1.50683E-02	-2.11330E-03	21	2.6012E+12	-4.84566E+04	1.00000
C2HO	8.24620E-14	9.36220E-09	-1.63594E-08	22	8.7238E+12	-4.48370E+04	0.99997
CH	2.29895E-12	2.60450E-07	-2.33637E-07	23	3.5548E+12	-2.89131E+05	0.99840
CO2	2.94490E-07	3.33630E-02	2.24375E-03	24	4.1951E+12	-6.01287E+04	1.00000
H2O2	1.00854E-11	1.14258E-06	-1.66092E-07	25	6.0000E+12	-3.24505E+03	0.99996
N2	6.47146E-06	7.33158E-01	-1.39162E-05	26	3.3000E+13	-6.17739E+04	1.00000
HCN	3.70069E-13	4.19255E-08	-2.92180E-08	27	5.0000E+12	-1.17527E+04	0.99996
N	1.07008E-12	1.21230E-07	1.50882E-08	28	3.0000E+13	-4.40179E+00	0.99115
CN	2.42331E-15	2.74539E-10	-1.86181E-10	29	3.0000E+13	-1.99072E-04	0.99923
HCNO	5.24095E-14	5.93752E-09	-1.41584E-09	30	6.8928E+06	-9.27869E+00	0.51982
NCO	1.58350E-14	1.79396E-09	-1.00964E-09	31	1.9939E+13	-1.16664E+05	0.99914
NH2	2.39470E-12	2.71298E-07	1.01137E-08	32	4.2387E+13	-1.19334E+05	0.99324
NO	6.36990E-10	7.21651E-05	2.77805E-05	33	1.4428E+12	1.81146E+03	0.95008
NH	6.78360E-14	7.68520E-09	1.22212E-09	34	3.6680E+11	-1.14685E+03	0.98770
NO2	4.20865E-13	4.76801E-08	1.94602E-08	35	3.6659E+13	-5.50197E+03	0.86475
N2O	6.50891E-12	7.37401E-07	1.75638E-08	36	2.0000E+13	-8.05112E+02	0.86453
HNO2	2.70052E-14	3.05944E-09	7.63746E-10	37	8.6245E+11	-8.52231E+04	1.00000
HNO3	3.13644E-18	3.55330E-13	9.72204E-14	38	1.2020E+12	-1.83268E+04	1.00000
HNO	9.25358E-14	1.04835E-08	1.98449E-09	39	1.0000E+13	-5.65020E+04	1.00000
				40	5.0000E+13	-6.47548E+04	0.87289
				41	3.0000E+13	-4.30850E+01	0.99998
				42	6.5630E+12	-2.90165E+00	0.99994
				43	1.0000E+13	-8.70650E-02	1.00000
				44	2.8000E+13	-2.00975E+04	0.99986
				45	5.9877E+12	-1.45773E+03	0.45025
				46	5.4903E+12	3.62811E+04	0.93782
				47	1.3915E+13	-1.86508E+02	0.44847
				48	9.2767E+12	-4.89658E+01	0.45039
				49	2.0000E+13	-7.12066E+04	1.00000
				50	6.5192E+10	-2.68353E+04	0.65700
				51	5.0000E+13	-2.61963E+03	0.99880
				52	2.2096E+12	-6.48701E+06	1.00000
				53	2.0000E+13	-7.88882E+06	1.00000
				54	1.9577E+09	4.81299E+05	0.99179
				55	2.3302E+13	-3.15263E+07	0.99980

TABLE D.2.—Continued.

(h) Concluded.

56	1.0791E+13	-2.02655E+06	0.99980
57	1.6714E+13	-6.9816E+06	0.99980
58	1.3820E+11	-7.49698E+02	0.99976
59	1.4666E+13	-2.99182E+04	0.99518
60	2.0000E+13	-1.23798E+06	0.79714
61	8.1934E+07	1.31009E+06	0.81871
62	2.2115E+11	1.03927E+06	0.99564
63	1.6821E+11	2.72626E+06	0.99566
64	2.2115E+11	-4.37970E+06	0.99565
65	3.7000E+12	-2.71234E+06	1.00000
66	1.0000E+13	-2.42006E+07	1.00000
67	5.6453E+12	-5.39733E+07	0.99999
68	2.0256E+11	-2.23498E+03	0.93021
69	7.0570E+12	-3.14433E+06	0.93020
70	2.6033E+13	-4.68386E+05	0.92997
71	5.0000E+12	-6.97522E+02	0.99981
72	4.0000E+13	-1.03379E+04	1.00000
73	3.0000E+13	-1.77206E+07	0.98129
74	3.0000E+13	-5.52331E+06	0.99604
75	3.0000E+13	-8.93434E+06	0.99604
76	2.0000E+13	-1.46561E+06	0.99602
77	1.0929E+13	2.36345E+07	0.83462
78	1.0122E+15	-2.7824E+08	0.98353
79	1.0885E+08	-5.56054E+05	0.31370
80	3.3782E+11	-8.84910E+08	0.31254
81	4.6003E+11	-9.06117E+06	0.85463
82	1.4226E+12	8.23685E+06	0.00025
83	5.9804E+12	1.06713E+08	0.00169
84	2.3219E+13	1.09010E+07	0.00348
85	4.6528E+13	-2.44673E+08	0.78744
86	4.0506E+13	-5.27725E+08	0.78818
87	8.0000E+12	-1.88176E+08	0.78813
88	1.0697E+14	-3.63733E+08	0.78854
89	4.0926E+11	-6.72749E+06	0.88377
90	4.5140E+12	-3.47400E+06	0.88415
91	1.8000E+12	-2.56925E+04	0.45321
92	7.8000E+11	-5.80603E+05	0.97550
93	9.9220E+12	-2.35229E+07	0.02159
94	1.3126E+13	-6.22577E+07	0.00323
95	1.8022E+15	-1.42386E+09	0.88687
96	3.1563E+05	-5.07962E+08	0.97603
97	2.9708E+15	-2.11259E+08	0.97604
98	3.6600E+05	-2.66489E+07	0.97595
99	1.2142E+04	-7.58392E+06	0.97600
100	1.8302E+09	1.50970E+03	1.00000
101	1.9655E+13	6.07974E+03	0.90889
102	7.9062E+11	1.06870E+04	0.90921
103	2.2182E+11	-2.71972E+03	0.94565
104	1.2000E+13	-4.18981E+03	0.99975
105	7.0673E+13	-5.50064E+03	0.54791
106	1.5031E+13	5.11157E+02	0.24211
107	1.6699E+13	-1.50819E+03	0.26818
108	2.5924E+13	-3.19571E+03	0.54868
109	3.7000E+12	2.65170E+01	0.34238
110	2.0000E+13	-6.06163E+04	0.99999
111	1.0000E+13	-5.05770E+01	0.99349
112	2.0000E+13	-8.22439E+03	0.99941
113	1.9730E+12	-1.97772E+03	1.00000
114	2.0000E+12	-3.56666E+03	0.99980
115	1.6042E+13	-7.38369E+03	0.07615
116	2.3108E+12	-2.49651E+02	0.01194
117	8.8206E+12	-2.50632E+05	0.78562
118	7.1749E+15	-4.90809E+06	0.88803
119	2.5463E+14	-1.79045E+06	0.78598
120	6.4580E+09	-7.04101E+06	0.97980
121	1.4962E+09	-2.73988E+06	0.97984
122	1.9161E+07	1.74320E+07	0.99831
123	4.0000E+12	-2.35361E+00	0.99568
124	2.8189E+09	-7.34631E+05	0.86997
125	2.7394E+11	-2.15135E+05	0.81540
126	2.5402E+11	-1.09650E+05	0.99999
127	3.1578E+12	-7.61702E+05	0.81571
128	5.3486E+10	-2.91988E+03	0.88751
129	6.6776E+15	-8.14530E+02	0.00003
130	8.0103E+15	-6.42917E+03	0.00113
131	5.0000E+12	-1.77807E+04	0.96366
132	6.1272E+15	-4.21056E+05	0.33831
133	3.6000E+13	-5.67397E+05	0.96378

DERIVATIVES (CGS UNITS): T 2.14301E+01 RHO -1.83017E-06 V 1.99510E+00
MIXTURE MOLECULAR WEIGHT 27.53632 TOTAL ENERGY EXCHANGE RATE -4.83687E+09 MASS FRACTION SUM 1.00000003
(CAL-CM**3/G**2/SEC)

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 5.949997E+00 S UP TO THIS TIME - 1.321999E+01 S

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS - 201
TOTAL NO. OF DERIVATIVE EVALUATIONS - 329
TOTAL NO. OF JACOBIAN EVALUATIONS - 42
TOTAL CPU TIME - 13.219994 S

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 15.500000 S

(LSENS) READ DATA FOR NEXT CASE

TABLE D.2.—Continued.

(i) Case 9

** DATA LINES **

1 2 3 4 5 6 7 8
 CC 123456789012345678901234567890123456789012345678901234567890

```

    LSENS  METHANE AIR MECHANISM  ASSIGNED (CONST.) TEMP. FLOW PROBLEM CASE 9
  REPEAT
  DISTANCE PRESSURE
    &prob  cx0=1.730, combus=.true., exchr=.false.,
    &print 25.0,42.0,48.0, &end
    &tmpdat cx0=1700.0, &end
    &start  area=1000.0, mach=2.0, &end
  CH4      0.049768
  O2       0.199072
  N2       0.75116
  CN       0.0000001
  END
  &solver  amax=1.0E-4, atolsp=1.0E-13, &end
  FINIS
  
```

** EQUILIBRIUM CALCULATION **

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED TEMPERATURE AND PRESSURE

	INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE (ATM)	1.7300	1.7300	1.0000
VELOCITY (CM/SEC)	0.00	0.00	1.0000
DENSITY (G/CM**3)	3.49869E-04	3.49843E-04	0.9999
TEMPERATURE (DEG K)	1700.00	1700.00	1.0000
ENTHALPY (CAL/G)	379.22696	41.16700	0.10856
INTERNAL ENERGY (CAL/G)	259.48010	-78.58891	-0.30287
SP. HEAT (CP) (CAL/G/DEG K)	0.32691	0.33141	1.01374
ENTROPY (CAL/G/DEG K)	2.1420	2.1511	1.0042
MACH NUMBER	0.0000	0.0000	1.0000
GAMMA	1.2746	1.2699	0.9963
SONIC VELOCITY (CM/SEC)	79913.95	79789.35	0.9984

SPECIES	MOLE FRACTION
CH4	2.82089E-10
CH3	2.82089E-10
H	2.43981E-07
H2	4.80198E-06
O2	9.84867E-02
HO2	9.40550E-07
O	1.05975E-05
OH	2.67611E-04
H2O	9.93892E-02
CH3O	2.82089E-10
CH2O	2.82089E-10
C2H6	2.82089E-10
C2H5	2.82089E-10
C2H4	2.82089E-10
CH2	2.82089E-10
C2H3	2.82089E-10
C2H2	2.82089E-10
HCN	2.82089E-10
C2H2O	2.82089E-10
C2H	2.82089E-10
CO	8.17330E-06
C2HO	2.82089E-10
CH	2.82089E-10
CO2	4.97562E-02
H2O2	2.40530E-08
N2	7.50131E-01
HCN	2.82089E-10
N	2.82089E-10
CN	2.82089E-10
HNCO	2.82089E-10
NCO	2.82089E-10
NH2	2.82089E-10
NO	1.93922E-03
NH	2.82089E-10
NO2	5.54534E-06
N2O	1.46579E-07
HNO2	8.25410E-08
HNO3	2.82089E-10
HNO	2.82089E-10

MIXTURE MOLECULAR WEIGHT	28.20888
D(LOG VOLUME)/D(LOG T) AT CONSTANT P	1.0010
D(LOG VOLUME)/D(LOG P) AT CONSTANT T	-1.0000

COMPUTATIONAL WORK REQUIRED FOR EQUILIBRIUM CALCULATION:
 NO. OF ITERATIONS = 23 CPU TIME = 8.000183E-02 S

TABLE D.2.—Continued.
(i) Continued.

** INITIAL CONDITIONS **									
TIME	0.00000E+00	SEC	AREA	1.00000E+03	SQ CM	AXIAL POSITION	0.00000E+00	CM	
FLOW PROPERTIES					INTEGRATION INDICATORS				
PRESSURE	1.73000				STEPS FROM LAST PRINT	0			
(ATM)					AVERAGE STEP SIZE	0.00000E+00			
VELOCITY	159827.88				METHOD ORDER	0			
(CM/SEC)									
DENSITY	5.49869E-04				TOTAL NUMBER OF STEPS	0			
(G/CM**3)					FUNCT EVALUATIONS	0			
TEMPERATURE	1700.00				JACOBIAN EVALUATIONS	0			
(DEG K)									
MASS FLOW RATE	5.59188E+04								
(G/SEC)									
ENTROPY	2.1420								
(CAL/G/DEG K)									
MACH NUMBER	2.0000								
GAMMA	1.2746								
ENTHALPY	5.79227E+02								
(CAL/G)									
SP. HEAT (CP)	5.26913E-01								
(CAL/G/DEG K)									
CHEMICAL PROPERTIES									
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST COS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR	POSITIVE DIR	RATE
CH4	6.17216E-07	4.97680E-02	-1.50903E-05	1	9.7244E+05	6.08103E+01	1.00000		
CH3	0.00000E+00	0.00000E+00	1.50903E-05	2	3.7198E+12	0.00000E+00	0.00000		
H	0.00000E+00	0.00000E+00	7.44369E-06	3	5.0180E+06	6.24678E+01	1.00000		
H2	0.00000E+00	0.00000E+00	0.00000E+00	4	5.9162E+12	0.00000E+00	0.00000		
O2	2.46886E-04	1.99072E-01	-8.05210E-05	5	5.6756E+12	0.00000E+00	0.00000		
H2O	0.00000E+00	0.00000E+00	7.64658E-06	6	4.9334E+09	0.00000E+00	0.00000		
O	0.00000E+00	0.00000E+00	7.28745E-05	7	6.3000E+12	0.00000E+00	0.00000		
DH	0.00000E+00	0.00000E+00	0.00000E+00	8	9.9825E+10	0.00000E+00	0.00000		
H2O	0.00000E+00	0.00000E+00	0.00000E+00	9	1.2247E+13	0.00000E+00	0.00000		
CH3O	0.00000E+00	0.00000E+00	0.00000E+00	10	7.4740E+12	0.00000E+00	0.00000		
CH2O	0.00000E+00	0.00000E+00	0.00000E+00	11	1.1064E+13	0.00000E+00	0.00000		
CH2H6	0.00000E+00	0.00000E+00	0.00000E+00	12	3.0690E+13	0.00000E+00	0.00000		
CH2H5	0.00000E+00	0.00000E+00	0.00000E+00	13	1.0344E+13	0.00000E+00	0.00000		
CH2H4	0.00000E+00	0.00000E+00	0.00000E+00	14	4.5524E+11	0.00000E+00	0.00000		
CH2	0.00000E+00	0.00000E+00	0.00000E+00	15	4.8000E+13	0.00000E+00	0.00000		
CH2H3	0.00000E+00	0.00000E+00	0.00000E+00	16	2.0000E+13	0.00000E+00	0.00000		
CH2H2	0.00000E+00	0.00000E+00	0.00000E+00	17	7.3247E+12	0.00000E+00	0.00000		
HCO	0.00000E+00	0.00000E+00	0.00000E+00	18	1.6606E+07	0.00000E+00	0.00000		
CH2H2O	0.00000E+00	0.00000E+00	0.00000E+00	19	3.3351E+12	0.00000E+00	0.00000		
CH2H	0.00000E+00	0.00000E+00	0.00000E+00	20	1.5053E+12	0.00000E+00	0.00000		
CO	0.00000E+00	0.00000E+00	0.00000E+00	21	2.3618E+12	0.00000E+00	0.00000		
CH2H	0.00000E+00	0.00000E+00	0.00000E+00	22	5.6904E+12	0.00000E+00	0.00000		
CH	0.00000E+00	0.00000E+00	0.00000E+00	23	2.3080E+11	0.00000E+00	0.00000		
CO2	0.00000E+00	0.00000E+00	0.00000E+00	24	4.2857E+12	0.00000E+00	0.00000		
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	25	6.0000E+12	0.00000E+00	0.00000		
N2	9.31578E-06	7.51160E-01	-1.20855E-11	26	3.3000E+13	0.00000E+00	0.00000		
HCN	0.00000E+00	0.00000E+00	0.00000E+00	27	5.0000E+12	0.00000E+00	0.00000		
N	0.00000E+00	0.00000E+00	0.00000E+00	28	3.0000E+13	0.00000E+00	0.00000		
CN	1.24019E-12	1.00000E-07	-7.28744E-05	29	3.0000E+13	0.00000E+00	0.00000		
HNC	0.00000E+00	0.00000E+00	0.00000E+00	30	7.3700E+02	0.00000E+00	0.00000		
HCO	0.00000E+00	0.00000E+00	7.28744E-05	31	8.5640E+12	0.00000E+00	0.00000		
NH2	0.00000E+00	0.00000E+00	0.00000E+00	32	1.7046E+13	0.00000E+00	0.00000		
NO	0.00000E+00	0.00000E+00	0.00000E+00	33	7.9329E+11	0.00000E+00	0.00000		
NH	0.00000E+00	0.00000E+00	0.00000E+00	34	3.0160E+11	0.00000E+00	0.00000		
NH2	0.00000E+00	0.00000E+00	0.00000E+00	35	3.2072E+13	0.00000E+00	0.00000		
N2O	0.00000E+00	0.00000E+00	1.20855E-11	36	2.0000E+13	0.00000E+00	0.00000		
HNO2	0.00000E+00	0.00000E+00	0.00000E+00	37	6.9656E+11	0.00000E+00	0.00000		
HNO3	0.00000E+00	0.00000E+00	0.00000E+00	38	1.2020E+12	0.00000E+00	0.00000		
HNO	0.00000E+00	0.00000E+00	0.00000E+00	39	1.0000E+13	0.00000E+00	0.00000		
				40	5.0000E+13	0.00000E+00	0.00000		
				41	3.0000E+13	0.00000E+00	0.00000		
				42	5.5320E+12	0.00000E+00	0.00000		
				43	1.0000E+13	0.00000E+00	0.00000		
				44	2.8000E+13	0.00000E+00	0.00000		
				45	3.0859E+12	0.00000E+00	0.00000		
				46	4.0962E+12	0.00000E+00	0.00000		
				47	7.0241E+12	0.00000E+00	0.00000		
				48	4.6827E+12	0.00000E+00	0.00000		
				49	2.0000E+13	0.00000E+00	0.00000		
				50	3.8682E+08	0.00000E+00	0.00000		
				51	5.0000E+13	0.00000E+00	0.00000		
				52	1.1974E+12	0.00000E+00	0.00000		
				53	2.0000E+13	0.00000E+00	0.00000		
				54	1.9307E+06	0.00000E+00	0.00000		
				55	2.1031E+13	0.00000E+00	0.00000		
				56	7.6735E+12	0.00000E+00	0.00000		
				57	1.2383E+13	0.00000E+00	0.00000		
				58	6.9803E+10	0.00000E+00	0.00000		
				59	1.2369E+13	0.00000E+00	0.00000		
				60	2.0000E+13	0.00000E+00	0.00000		
				61	5.2663E+04	0.00000E+00	0.00000		
				62	1.9580E+10	0.00000E+00	0.00000		
				63	1.4842E+10	0.00000E+00	0.00000		
				64	1.9580E+10	0.00000E+00	0.00000		
				65	3.7000E+12	0.00000E+00	0.00000		
				66	1.0000E+13	0.00000E+00	0.00000		
				67	2.6268E+12	0.00000E+00	0.00000		
				68	1.7601E+10	0.00000E+00	0.00000		
				69	3.5950E+12	0.00000E+00	0.00000		
				70	1.3413E+13	0.00000E+00	0.00000		
				71	5.0000E+12	0.00000E+00	0.00000		
				72	4.0000E+13	0.00000E+00	0.00000		
				73	3.0000E+13	0.00000E+00	0.00000		
				74	3.0000E+13	0.00000E+00	0.00000		
				75	3.0000E+13	0.00000E+00	0.00000		
				76	2.0000E+13	0.00000E+00	0.00000		
				77	2.8889E+12	0.00000E+00	0.00000		
				78	7.1505E+14	0.00000E+00	0.00000		

TABLE D.2.—Continued.

(i) Continued.

79	1.8492E+06	0.00000E+00	0.00000
80	3.1015E+11	0.00000E+00	0.00000
81	6.4836E+10	0.00000E+00	0.00000
82	2.9616E+11	0.00000E+00	0.00000
83	1.4726E+12	0.00000E+00	0.00000
84	7.1708E+12	0.00000E+00	0.00000
85	3.8799E+13	0.00000E+00	0.00000
86	3.7189E+13	0.00000E+00	0.00000
87	8.0000E+12	0.00000E+00	0.00000
88	9.7622E+13	0.00000E+00	0.00000
89	4.8329E+10	0.00000E+00	0.00000
90	3.9948E+12	0.00000E+00	0.00000
91	1.8000E+12	0.00000E+00	0.00000
92	7.8000E+11	0.00000E+00	0.00000
93	2.0307E+11	0.00000E+00	0.00000
94	7.7952E+12	0.00000E+00	0.00000
95	1.9630E+15	0.00000E+00	0.00000
96	3.9562E+01	0.00000E+00	0.00000
97	4.1765E+15	0.00000E+00	0.00000
98	1.0018E+02	0.00000E+00	0.00000
99	7.1175E-01	1.78032E-04	1.00000
100	3.6090E+08	0.00000E+00	0.00000
101	1.2497E+13	0.00000E+00	0.00000
102	1.4798E+11	0.00000E+00	0.00000
103	1.7462E+11	0.00000E+00	0.00000
104	1.2000E+13	0.00000E+00	0.00000
105	4.2324E+13	0.00000E+00	0.00000
106	6.9658E+12	0.00000E+00	0.00000
107	8.0770E+12	0.00000E+00	0.00000
108	2.3801E+13	5.95338E+02	1.00000
109	3.7000E+12	0.00000E+00	0.00000
110	2.0000E+13	0.00000E+00	0.00000
111	1.0000E+13	0.00000E+00	0.00000
112	2.0000E+13	0.00000E+00	0.00000
113	8.4381E+11	0.00000E+00	0.00000
114	2.0000E+12	0.00000E+00	0.00000
115	1.1405E+13	0.00000E+00	0.00000
116	2.4070E+12	0.00000E+00	0.00000
117	8.3826E+12	0.00000E+00	0.00000
118	7.9225E+15	0.00000E+00	0.00000
119	2.2457E+14	0.00000E+00	0.00000
120	8.6958E+07	0.00000E+00	0.00000
121	3.1028E+07	0.00000E+00	0.00000
122	2.8358E+04	0.00000E+00	0.00000
123	4.0000E+12	0.00000E+00	0.00000
124	2.5566E+07	0.00000E+00	0.00000
125	2.4991E+10	-9.87306E-05	1.00000
126	2.6097E+10	0.00000E+00	0.00000
127	8.8897E+11	0.00000E+00	0.00000
128	4.4875E+09	0.00000E+00	0.00000
129	9.2394E+15	0.00000E+00	0.00000
130	9.2627E+15	0.00000E+00	0.00000
131	5.0000E+12	0.00000E+00	0.00000
132	6.4495E+15	0.00000E+00	0.00000
133	3.6000E+13	0.00000E+00	0.00000

DERIVATIVES (CGS UNITS): T 0.00000E+00 RHO -1.31388E-09 V 0.00000E+00
 MIXTURE MOLECULAR WEIGHT 28.21102 TOTAL ENERGY EXCHANGE RATE 5.92105E+06 MASS FRACTION SUM 1.00000000
 (CAL-CM**3/G**2/SEC)

CPU TIME FOR INITIALIZATION OF LSENS = 1.190010 S

TIME 3.00323E-04 SEC AREA 1.00533E+03 SQ CM AXIAL POSITION 4.80000E+01 CM

FLOW PROPERTIES

PRESSURE 1.73000
 (ATM)
 VELOCITY 159827.88
 (CM/SEC)
 DENSITY 3.48013E-04
 (G/CM**3)
 TEMPERATURE 1700.00
 (DEG K)
 MASS FLOW RATE 5.59188E+04
 (G/SEC)
 ENTROPY 2.1620
 (CAL/G/DEG K)
 MACH NUMBER 1.9915
 GAMMA 1.2787
 ENTHALPY 3.22341E+02
 (CAL/O)
 SP. HEAT (CP) 3.24936E-01
 (CAL/G/DEG K)

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 6
 AVERAGE STEP SIZE 0.10519E+01
 METHOD ORDER 4
 TOTAL NUMBER OF STEPS 137
 FUNCT EVALUATIONS 184
 JACOBIAN EVALUATIONS 25

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST COS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
CH4	2.88178E-07	2.32367E-02	-2.67162E-03	2	9.7244E+05	-1.35854E+02	0.82561
CH3	1.91140E-08	1.54122E-03	6.04892E-06	2	3.7198E+12	1.98822E+03	0.72567
H	3.09554E-10	2.49603E-05	4.69517E-06	3	5.0180E+06	-2.16252E+02	0.89255
H2	2.98194E-08	2.40443E-03	2.39713E-04	4	5.9162E+12	5.33818E+03	0.99295
O2	2.18046E-06	1.75817E-01	-3.02746E-03	5	5.6736E+12	1.55999E+04	0.95284
H02	3.45739E-09	2.78780E-04	1.33554E-05	6	4.9334E+09	1.63935E+03	0.96563
O	3.81901E-10	3.07938E-05	5.71794E-06	7	6.3000E+12	-5.92180E+03	0.83083
OH	1.21275E-09	9.77881E-05	1.69045E-05	8	9.9825E+10	2.13057E+03	1.00000
H2O	3.78990E-07	3.05592E-02	4.30922E-03	9	1.2247E+13	8.16156E+03	0.22092
CH3O	2.08432E-10	1.68065E-05	-5.14536E-07	10	7.4740E+12	4.52179E+02	0.99990
CH2O	4.37161E-08	3.52496E-03	-1.69220E-04	11	1.1064E+13	8.25857E+02	1.00000
C2H6	2.36730E-08	1.90883E-03	-4.73879E-05	12	3.0690E+13	7.27479E+03	0.99998

TABLE D.2.—Continued.

(i) Continued.

C2H5	9.88112E-12	7.96745E-07	1.58219E-07	13	1.0344E+13	8.49427E+03	0.81160
C2H4	4.70382E-08	3.79284E-03	5.12019E-04	14	4.5524E+11	5.62227E+01	0.69424
CH2	1.79722E-11	1.44916E-06	5.07118E-07	15	4.8000E+13	1.20132E+00	0.99099
C2H3	2.42732E-11	1.95723E-06	6.49998E-07	16	2.0000E+13	5.67153E+01	0.99979
C2H2	2.30923E-09	1.86200E-04	5.30853E-05	17	7.3247E+12	8.79821E+02	0.99909
MCU	1.72899E-11	1.39414E-06	2.03886E-07	18	1.6606E+07	7.99856E+01	0.99999
C2H2O	1.96327E-11	1.58304E-06	5.91704E-07	19	3.3351E+12	1.57065E+03	0.99984
C2H	3.13259E-14	2.52590E-09	1.47195E-09	20	1.5053E+12	6.56109E+02	0.92540
CO	1.13925E-07	9.18610E-03	1.72638E-03	21	2.3618E+12	3.50311E+02	1.00000
C2HO	1.07987E-11	8.70729E-07	4.19384E-07	22	5.6904E+12	8.43917E+02	0.99987
CH	6.98679E-15	5.63364E-10	3.47858E-10	23	2.3080E+11	5.68072E+02	0.99023
CO2	2.59512E-09	2.09253E-04	6.91888E-05	24	4.2857E+12	1.87287E+03	1.00000
H2O2	9.50117E-12	7.66109E-07	6.55731E-08	25	6.0000E+12	3.72067E-01	0.99953
N2	9.26636E-06	7.47175E-01	-1.72464E-09	26	3.3000E+13	2.52581E+00	1.00000
HCN	2.55361E-15	2.05905E-10	4.97298E-11	27	5.0000E+12	1.21519E+00	0.99992
N	7.78540E-17	6.27760E-12	7.50689E-13	28	3.0000E+13	1.07325E-01	0.99321
CN	3.20665E-18	2.58562E-13	6.29686E-13	29	3.0000E+13	1.87195E-04	0.99388
HNCO	9.54948E-13	7.70004E-08	-2.18034E-09	30	7.3700E+02	-1.03774E-04	0.37322
HCO	1.44339E-15	1.16385E-10	4.35551E-12	31	8.5640E+12	6.23591E-12	1.00000
HN2	1.62101E-13	1.30707E-08	2.12906E-09	32	1.7046E+13	1.24122E+02	0.99999
HU	1.05015E-13	8.46765E-09	4.81276E-10	33	7.9329E+11	1.81026E+01	0.98688
HN	1.33005E-14	1.07246E-09	-1.74864E-10	34	3.0160E+11	6.97369E+00	0.99995
H2O	1.16014E-14	9.35452E-10	-6.06635E-11	35	3.2072E+13	1.80878E+01	0.99998
H2D	1.33764E-13	1.07860E-08	1.59959E-09	36	2.0000E+13	6.25400E-03	0.99688
HN2O	1.80283E-18	1.45368E-13	3.08435E-14	37	6.9656E+11	1.35420E+02	1.00000
HN2O3	2.81432E-20	2.26928E-15	2.14810E-16	38	1.2020E+12	4.09293E-02	1.00000
HN2O	7.99676E-18	6.44803E-13	1.56210E-13	39	1.0000E+13	1.08131E+00	1.00000
				40	5.0000E+13	1.35345E+00	0.98075
				41	3.0000E+13	4.80731E-02	1.00000
				42	5.5320E+12	8.81928E-03	0.99688
				43	1.0000E+13	9.62829E-03	1.00000
				44	2.8000E+13	4.79306E+00	0.87075
				45	5.0859E+12	1.50609E+01	0.24826
				46	4.0962E+12	-4.57247E-02	0.18194
				47	7.0241E+12	-1.18874E+00	0.77131
				48	4.6827E+12	2.57325E-01	0.88765
				49	2.0000E+13	1.23814E+00	1.00000
				50	3.8682E+08	-5.90714E-01	0.43169
				51	5.0000E+13	4.93893E-03	1.00000
				52	1.1974E+12	4.49318E+03	0.99999
				53	2.0000E+13	1.06347E+01	1.00000
				54	1.9507E+06	8.63618E+00	0.99924
				55	2.1031E+13	9.20600E+03	0.99999
				56	7.6735E+12	8.57356E+02	0.99996
				57	1.2383E+13	1.70697E+03	1.00000
				58	6.9803E+10	4.81523E+02	0.99987
				59	1.2369E+13	3.37507E+01	0.99996
				60	2.0000E+13	1.09126E+04	0.99997
				61	3.2663E+04	-2.80915E-02	0.30527
				62	1.9580E+10	8.90671E-01	0.93114
				63	1.4842E+10	8.92983E-01	0.99823
				64	1.9580E+10	3.70312E+00	0.98816
				65	3.7000E+12	5.53889E-04	0.99995
				66	1.0000E+13	1.25787E+00	1.00000
				67	2.6268E+12	8.49934E+02	1.00000
				68	1.7601E+10	9.97184E-04	0.99973
				69	3.5950E+12	6.45812E-01	0.99822
				70	1.3413E+13	6.09738E-01	0.98962
				71	5.0000E+12	1.33347E-02	1.00000
				72	4.0000E+13	1.06678E-01	1.00000
				73	3.0000E+13	9.33507E+03	0.99965
				74	3.0000E+13	1.6558E+00	1.00000
				75	3.0000E+13	5.19391E+00	1.00000
				76	2.0000E+13	8.83818E-01	0.99999
				77	2.8889E+12	5.11367E+03	0.99978
				78	7.1305E+14	3.17676E+00	1.00000
				79	1.8492E+06	3.79270E+00	0.99999
				80	3.1015E+11	3.53445E+02	0.99895
				81	6.4836E+110	2.10859E+02	1.00000
				82	2.9616E+11	3.01034E+02	0.81055
				83	1.4726E+12	8.15945E+03	0.99419
				84	7.1708E+12	6.56932E+02	0.97431
				85	3.8799E+13	3.32748E+02	0.91052
				86	3.7189E+13	4.05126E+02	0.99924
				87	8.0000E+12	2.75559E+02	0.99493

TABLE D.2.—Continued.
(i) Concluded.

88	9.7622E+13	8.62659E+02	1.00000
89	4.8329E+10	4.02368E+01	0.97804
90	3.9948E+12	-2.59592E+00	0.87229
91	1.8000E+12	1.77541E+02	0.99915
92	7.8000E+11	1.89410E-02	0.99997
93	2.0307E+11	2.19815E+02	0.99581
94	7.7952E+12	1.92744E+03	0.82808
95	1.9630E+15	-1.60454E+02	0.38383
96	3.9562E+01	-3.79522E-01	0.99178
97	4.1765E+15	5.04961E-02	0.99877
98	1.0018E+02	-1.43576E-02	0.95216
99	7.1175E-01	-5.92715E-04	0.78857
100	3.6090E+08	1.92921E-04	1.00000
101	1.2497E+13	8.63664E-06	0.87558
102	1.4798E+11	9.45868E-07	0.79383
103	1.7462E+11	-2.09982E-04	0.97918
104	1.2000E+13	1.21336E-07	1.00000
105	4.2324E+13	-6.12937E-06	0.81852
106	6.9658E+12	-2.13415E-04	0.07937
107	8.0770E+12	1.75791E-02	0.89171
108	2.3801E+15	1.33002E-03	0.96796
109	3.7000E+12	-1.33691E-03	0.99981
110	2.0000E+15	9.10278E-05	1.00000
111	1.0000E+13	9.27635E-12	0.99978
112	2.0000E+13	7.34138E-05	0.99499
113	8.4381E+11	5.11150E-09	0.99992
114	2.0000E+12	1.21159E-08	0.99998
115	1.1405E+13	1.51722E-03	0.99890
116	2.4070E+12	6.87200E-03	0.95237
117	8.3826E+12	3.01776E-04	0.98410
118	7.9225E+15	-4.00037E-04	0.92479
119	2.2457E+14	6.65828E-03	0.99991
120	8.6958E+07	-3.29896E-05	0.99929
121	3.1028E+07	-2.49967E-03	1.00000
122	2.8358E+04	8.28589E-04	1.00000
123	4.0000E+12	2.98303E-11	1.00000
124	2.5566E+07	-1.34240E-02	0.97458
125	2.4991E+10	-7.71212E-05	0.87975
126	2.6097E+10	1.10076E-05	1.00000
127	8.6897E+11	2.82732E-04	0.95165
128	4.4875E+09	1.27908E-05	0.99787
129	9.2394E+15	1.77363E-09	0.00014
130	9.2627E+15	-1.25361E-05	0.09402
131	5.0000E+12	9.61607E-08	0.94095
132	6.4495E+15	4.07424E-06	0.18977
133	3.6000E+13	2.85345E-06	0.98985
DERIVATIVES (CGS UNITS), T			
0.00000E+00 RHO			
-1.83068E-07 V			
0.00000E+00			
MIXTURE MOLECULAR WEIGHT			
28.06136			
TOTAL ENERGY EXCHANGE RATE			
(CAL-CM**3/G**2/SEC)			
-1.95990E+09			
MASS FRACTION SUM			
1.00000001			

COMPUTER TIME (CPU) REQUIRED, FOR THIS STEP - 3.499985E-01 S UP TO THIS TIME - 6.219994E+00 S

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM.

TOTAL NO. OF STEPS - 137
TOTAL NO. OF DERIVATIVE EVALUATIONS - 184
TOTAL NO. OF JACOBIAN EVALUATIONS - 25
TOTAL CPU TIME - 6.219994 S

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 8.700005 S

(LSENS) READ DATA FOR NEXT CASE

TABLE D.2.—Continued

(j) Case 10

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM										NASA LEWIS RESEARCH CENTER	
LESENS METHANOL - AIR COMBUSTION										CASE 10	
REACTION NUMBER	REACTION					REACTION RATE A	VARIABLES N	ACTIVATION ENERGY			
1	M	+ 1*CH3OH	= 1*CH3	+	1*OH	3.20000E+18	0.0000	80000.00			
2	1*O2	+ 1*CH3OH	= 1*CH2OH	+	1*HO2	4.00000E+13	0.0000	50900.00			
3	1*OH	+ 1*CH3OH	= 1*CH2OH	+	1*H2O	0.00000E+12	0.0000	2000.00			
4	1*O	+ 1*CH3OH	= 1*CH2OH	+	1*OH	1.60000E+12	0.0000	2300.00			
5	1*H	+ 1*CH3OH	= 1*CH2OH	+	1*H2	3.20000E+13	0.0000	7000.00			
6	1*H	+ 1*CH3OH	= 1*CH3	+	1*H2O	5.00000E+12	0.0000	5300.00			
7	1*CH3	+ 1*CH3OH	= 1*CH2OH	+	1*CH4	2.00000E+11	0.0000	9800.00			
8	1*HO2	+ 1*CH3OH	= 1*CH2OH	+	1*H2O2	6.30000E+12	0.0000	19400.00			
9	M	+ 1*CH2OH	= 1*CH2O	+	1*H	2.50000E+13	0.0000	29000.00			
10	1*O2	+ 1*CH2OH	= 1*CH2O	+	1*HO2	1.00000E+12	0.0000	6000.00			
11	M	+ 1*CH4	= 1*CH3	+	1*H	2.00000E+17	0.0000	88000.00			
12	1*H	+ 1*CH4	= 1*CH3	+	1*H2	1.26000E+14	0.0000	11900.00			
13	1*CH4	+ 1*O2	= 1*CH3	+	1*HO2	7.94000E+13	0.0000	56000.00			
14	1*O	+ 1*CH4	= 1*CH3	+	1*OH	1.90000E+14	0.0000	11720.00			
15	1*OH	+ 1*CH4	= 1*CH3	+	1*H2O	2.50000E+13	0.0000	5010.00			
16	1*CH3	+ 1*O2	= 1*CH3O	+	1*O	2.40000E+13	0.0000	28680.00			
17	1*CH3	+ 1*OH	= 1*CH3O	+	1*H	6.30000E+12	0.0000	0.00			
18	M	+ 1*CH3O	= 1*CH2O	+	1*H	5.00000E+13	0.0000	21000.00			
19		2*CH3	= 1*CH2H6			2.40000E+14	0.4000	0.00			
20	1*H	+ 1*CH2H6	= 1*CH2H5	+	1*H2	1.32000E+14	0.0000	9700.00			
21	1*O	+ 1*CH2H6	= 1*CH2H5	+	1*OH	1.15000E+14	0.0000	7850.00			
22	1*OH	+ 1*CH2H6	= 1*CH2H5	+	1*H2O	8.70000E+13	0.0000	3520.00			
23	M	+ 1*CH2H5	= 1*CH2H4	+	1*H	1.00000E+17	0.0000	51000.00			
24	1*CH2H5	+ 1*O2	= 1*CH2H4	+	1*HO2	2.00000E+12	0.0000	5000.00			
25	1*H	+ 1*CH2H5	= 1*CH2H4	+	1*H2	4.80000E+13	0.0000	0.00			
26	1*CH3	+ 1*CH2	= 1*CH2H4	+	1*H	2.00000E+13	0.0000	0.00			
27	1*H	+ 1*CH2H4	= 1*H2	+	1*CH2H3	1.50000E+14	0.0000	10200.00			
28	M	+ 1*CH2H4	= 1*CH2H2	+	1*H2	2.60000E+17	0.0000	79300.00			
29	1*CH2H4	+ 1*OH	= 1*CH2H3	+	1*H2O	4.80000E+12	0.0000	1250.00			
30	1*CH2H4	+ 1*OH	= 1*CH3	+	1*CH2O	2.00000E+12	0.0000	960.00			
31	1*CH2H4	+ 1*O	= 1*HCO	+	1*HCO	3.30000E+13	0.0000	1130.00			
32	1*CH2H4	+ 1*O	= 1*CH2O	+	1*CH2	2.50000E+13	0.0000	5000.00			
33	M	+ 1*CH2H3	= 1*CH2H2	+	1*H	3.00000E+15	0.0000	52000.00			
34	1*CH2H3	+ 1*O2	= 1*CH2H2	+	1*HCO	3.98000E+12	0.0000	-250.00			
35	1*CH2H3	+ 1*H	= 1*CH2H2	+	1*H2	6.00000E+12	0.0000	0.00			
36	1*CH2H3	+ 1*O	= 1*CH2H2O	+	1*H	3.30000E+13	0.0000	0.00			
37	1*CH2H3	+ 1*OH	= 1*CH2H2	+	1*H2O	5.00000E+12	0.0000	0.00			
38	1*CH2H3	+ 1*CH2	= 1*CH2H2	+	1*CH3	3.00000E+13	0.0000	0.00			
39	1*CH2H3	+ 1*CH2H	= 2*CH2H2			3.00000E+13	0.0000	0.00			
40	M	+ 1*CH2H2	= 1*CH2H	+	1*H	4.20000E+16	0.0000	107000.00			
41	1*CH2H2	+ 1*O	= 1*CH2	+	1*CO	1.60000E+14	0.0000	9890.00			
42	1*CH2H2	+ 1*O	= 1*CH2H	+	1*H	4.00000E+14	0.0000	10660.00			
43	1*CH2H2	+ 1*OH	= 1*CH2H	+	1*H2O	6.30000E+12	0.0000	7000.00			
44	1*CH2H2	+ 1*OH	= 1*CH2H2O	+	1*H	3.20000E+11	0.0000	200.00			
45	1*CH2H	+ 1*O2	= 1*CH2H	+	1*O	5.00000E+13	0.0000	1500.00			
46	1*CH2H	+ 1*OH	= 1*CH2H	+	1*H	2.00000E+13	0.0000	0.00			
47	1*CH2H	+ 1*O2	= 2*CO	+	1*OH	1.46000E+12	0.0000	2500.00			
48	1*CH2H	+ 1*O	= 2*CO	+	1*H	1.20200E+12	0.0000	0.00			
49	1*CH2H	+ 1*OH	= 2*HCO			1.00000E+13	0.0000	0.00			
50	1*CH2H	+ 1*H	= 1*CH2	+	1*CO	5.00000E+13	0.0000	0.00			
51	1*CH2H	+ 1*CH2	= 1*CH2H3	+	1*CO	3.00000E+13	0.0000	0.00			
52	1*CH2H	+ 1*CH2	= 1*CH2H	+	1*CH2H	1.00000E+13	0.0000	2000.00			
53		2*CH2H	= 1*CH2H	+	2*CO	1.00000E+13	0.0000	0.00			
54	1*CH2H2O	+ 1*OH	= 1*CH2H	+	1*HCO	2.80000E+13	0.0000	0.00			
55	1*CH2H2O	+ 1*OH	= 1*CH2H	+	1*H2O	7.50000E+12	0.0000	3000.00			
56	1*CH2H2O	+ 1*H	= 1*CH3	+	1*CO	1.15000E+13	0.0000	3428.00			
57	1*CH2H2O	+ 1*H	= 1*CH2H	+	1*H2	7.50000E+13	0.0000	8000.00			
58	1*CH2H2O	+ 1*O	= 1*CH2H	+	1*OH	5.00000E+13	0.0000	8000.00			
59	1*CH2H2O	+ 1*O	= 1*CH2H	+	1*CO	2.00000E+13	0.0000	0.00			
60	M	+ 1*CH2H2O	= 1*CH2	+	1*CO	2.00000E+16	0.0000	60000.00			
61	1*CH2H	+ 1*O	= 1*CO	+	1*CH	5.00000E+13	0.0000	0.00			
62	1*CH3O	+ 1*O2	= 1*CH2O	+	1*HO2	1.00000E+13	0.0000	7170.00			
63	1*CH3O	+ 1*H	= 1*CH2O	+	1*H2	2.00000E+13	0.0000	0.00			
64	M	+ 1*CH2O	= 1*HCO	+	1*H	5.00000E+16	0.0000	81000.00			
65	1*CH2O	+ 1*OH	= 1*HCO	+	1*H2O	3.00000E+13	0.0000	1200.00			
66	1*CH2O	+ 1*H	= 1*HCO	+	1*H2	2.50000E+15	0.0000	3990.00			
67	1*CH2O	+ 1*O	= 1*HCO	+	1*OH	5.00000E+13	0.0000	3510.00			
68	1*CH3	+ 1*CH2O	= 1*CH4	+	1*HCO	1.00000E+10	0.5000	6000.00			
69	1*CH3	+ 1*HCO	= 1*CH4	+	1*CO	3.00000E+11	0.5000	0.00			
70	1*CH3	+ 1*HO2	= 1*CH3O	+	1*OH	2.00000E+13	0.0000	0.00			
71	M	+ 1*CH2	= 1*CH2	+	1*H	1.95000E+16	0.0000	91600.00			
72	1*H	+ 1*CH3	= 1*H2	+	1*CH2	2.70000E+11	0.6700	25700.00			
73	1*O	+ 1*CH3	= 1*OH	+	1*CH2	1.90000E+11	0.6800	25700.00			
74	1*OH	+ 1*CH3	= 1*H2O	+	1*CH2	2.70000E+11	0.6700	25700.00			
75	1*CH	+ 1*CO2	= 1*HCO	+	1*CO	3.70000E+12	0.0000	0.00			
76	1*CH	+ 1*O2	= 1*HCO	+	1*O	1.00000E+13	0.0000	0.00			
77	1*CH2	+ 1*O2	= 1*CH2O	+	1*O	5.00000E+11	0.5000	6960.00			
78	1*CH2	+ 1*O	= 1*CH	+	1*OH	2.00000E+11	0.7000	25800.00			
79	1*CH2	+ 1*OH	= 1*CH	+	1*H2O	5.00000E+11	0.5000	5900.00			
80	1*CH2	+ 1*H	= 1*CH	+	1*H2	3.20000E+11	0.7000	4970.00			
81		2*CH2	= 1*CH2H3	+	1*H	5.00000E+12	0.0000	0.00			
82		2*CH2	= 1*CH2H2	+	1*H2	4.00000E+13	0.0000	0.00			
83	1*HCO	+ 1*O2	= 1*CO	+	1*HO2	3.00000E+13	0.0000	0.00			
84	1*HCO	+ 1*O	= 1*CO	+	1*OH	5.00000E+13	0.0000	0.00			
85	1*HCO	+ 1*OH	= 1*CO	+	1*H2O	5.00000E+13	0.0000	0.00			
86	1*HCO	+ 1*H	= 1*CO	+	1*H2	2.00000E+13	0.0000	0.00			
87	M	+ 1*HCO	= 1*H	+	1*CO	2.90000E+14	0.0000	15570.00			
88	1*O	+ 1*CO2	= 1*O	+	1*H	2.40000E+15	0.0000	4100.00			
89	1*CO	+ 1*O2	= 1*CO2	+	1*O	2.50000E+12	0.0000	47690.00			
90	1*CO	+ 1*OH	= 1*CO2	+	1*H	4.17000E+11	0.0000	1000.00			
91	1*CO	+ 1*HO2	= 1*CO2	+	1*OH	5.75000E+13	0.0000	22930.00			
92	1*O	+ 1*H2O	= 2*OH			6.80000E+13	0.0000	18365.00			
93	1*H	+ 1*O2	= 1*OH	+	1*O	1.69000E+14	0.0000	16400.00			
94	1*O	+ 1*H2	= 1*OH	+	1*H	4.20000E+14	0.0000	13750.00			
95	1*H	+ 1*HO2	= 1*H2	+	1*O2	7.28000E+13	0.0000	2126.00			
96	1*O	+ 1*HO2	= 1*OH	+	1*O2	5.00000E+13	0.0000	1000.00			
97	1*HO2	+ 1*OH	= 1*H2O	+	1*O2	8.00000E+12	0.0000	0.00			
98	1*H	+ 1*HO2	= 2*OH			1.34000E+14	0.0000	1070.00			
99	1*OH	+ 1*HO2	= 1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00			
100	1*HO2	+ 1*H2O2	= 1*H2O	+	1*HO2	6.10000E+12	0.0000	1430.00			
101		2*H2O2	= 1*H2O2	+	1*O2	1.80000E+12	0.0000	0.00			
102	1*H	+ 1*H2O2	= 1*OH	+	1*H2O	7.80000E+17	0.0000	0.00			
103	M	+ 1*H2O2	= 2*OH			1.44000E+17	0.0000	45510.00			
104	1*H2	+ 1*OH	= 1*H2O	+	1*H	4.74000E+13	0.0000	6098.00			

TABLE D.2.—Continued.

(j) Continued.

105	1KH	+	1K02	=	1KH02	+	M	1.46000E+15	0.0000	-1000.00
106	M	+	1KH20	=	1KH	+	1KH0H	1.30000E+15	0.0000	105140.00
107	1KH	+	1K0	=	1KH0H	+	M	7.10000E+18	-1.0000	0.00
108	M	+	1KH2	=	2KH			2.20000E+14	0.0000	96000.00
109	M	+	1K02	=	2K0			1.80000E+18	-1.0000	118020.00
110	1KCH	+	1KH2	=	1KHCH	+	1KH	1.00000E+11	0.0000	19000.00
111	1KCH	+	1KH2	=	1KHCH	+	1KH	6.00000E+13	0.0000	5300.00
112	1K0	+	1KHCH	=	1KH0H	+	1KHCH	1.40000E+11	0.6800	16900.00
113	1KH0H	+	1KHCH	=	1KHCHCO	+	1KH	4.00000E+11	0.0000	2800.00
114	1KCH	+	1K0	=	1KCO	+	1KH	1.20000E+13	0.0000	0.00
115	1KCH	+	1KH0H	=	1KHCO	+	1KH	2.50000E+14	0.0000	6000.00
116	1KH2	+	1KHCO	=	1KHCHCO	+	1KH	1.00000E+14	0.0000	9000.00
117	1KHCHCO	+	1KH	=	1KHCH2	+	1KCO	1.00000E+14	0.0000	8500.00
118	1KCH	+	1K02	=	1KHCO	+	1K0	3.20000E+13	0.0000	1000.00
119	1KCH	+	1KCO2	=	1KHCO	+	1KCO	3.70000E+12	0.0000	0.00
120	1K0	+	1KHCO	=	1KH0	+	1KCO	2.00000E+13	0.0000	0.00
121	1KH	+	1KHCO	=	1KH2	+	1KCO	1.00000E+13	0.0000	0.00
122	1KH	+	1KHCO	=	1KHCH	+	1KCO	2.00000E+13	0.0000	0.00
123	1KCH	+	1KH0	=	1KH	+	1KHCO	1.60000E+13	0.0000	0.00
124	1KCH	+	1KH0	=	1K0	+	1KHCH	2.00000E+12	0.0000	9940.00
125	1KHCH	+	1KH0H	=	1KH	+	1KH20	5.00000E+11	0.5000	2000.00
126	1KH02	+	1KH0	=	1KH02	+	1KH0H	2.09000E+12	0.0000	-477.00
127	1K0	+	1KH02	=	1KH0	+	1K02	1.00000E+13	0.0000	596.00
128	1KH0	+	1K0	=	1KH02	+	M	5.62000E+15	0.0000	-1160.00
129	1KH02	+	1KH	=	1KH0	+	1KH0H	3.47000E+14	0.0000	1470.00
130	1KH0	+	1KH	=	1KH	+	1KH0H	2.63000E+14	0.0000	50410.00
131	1KH0	+	1K0	=	1KH	+	1K02	3.80000E+09	1.0000	41370.00
132	1K0	+	1KH2	=	1KH0	+	1KH	1.80000E+14	0.0000	76250.00
133	1KH	+	1KH02	=	2KH0			4.00000E+12	0.0000	0.00
134	M	+	1KH20	=	1KH2	+	1K0	6.92000E+23	-2.5000	65000.00
135	1KH0	+	1KH20	=	1KH2	+	1K02	1.00000E+14	0.0000	28020.00
136	1K0	+	1KH20	=	2KH0			6.92000E+13	0.0000	26630.00
137	1KH20	+	1KH	=	1KH2	+	1KH0H	7.59000E+13	0.0000	15100.00
138	1KH02	+	1KH2	=	1KH02	+	1KH	2.40000E+13	0.0000	29000.00
139	1KH0H	+	1KH02	=	1KH03	+	M	3.00000E+15	0.0000	-3800.00
140	1KH0H	+	1KH0	=	1KH02	+	M	5.60000E+15	0.0000	-1700.00
141	1KH0	+	1KH	=	1KH2	+	1KH0	5.00000E+12	0.0000	0.00
142	1KH	+	1KH0	=	1KH0	+	M	5.40000E+15	0.0000	-600.00
143	1KH0	+	1KH0H	=	1KH20	+	1KH0	3.60000E+13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	,103) = 2.30000	M(O2	,103) = 0.78000	M(H20	,103) = 6.00000	M(H202	,103) = 6.60000
M(O2	,105) = 1.30000	M(H2	,105) = 1.30000	M(H20	,105) = 21.30000	M(CO2	,105) = 7.00000
M(H2	,106) = 4.00000	M(O2	,106) = 1.50000	M(H20	,106) = 20.00000	M(H2	,106) = 1.50000
M(CO2	,106) = 4.00000	M(H2	,108) = 4.10000	M(O2	,108) = 2.00000	M(H20	,108) = 15.00000
M(H2	,108) = 2.00000	M(O2	,139) = 0.70000	M(H2	,139) = 1.40000		

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE 1.00000
(ATM)
VELOCITY 0.00
(CM/SEC)
DENSITY 2.77826E-04
(G/CM**3)
TEMPERATURE 1300.00
(DEG K)
MASS FLOW RATE 0.00000E+00
(G/SEC)
ENTROPY 2.1788
(CAL/G/DEG K)
MACH NUMBER 0.0000
GAMMA 1.2066
ENTHALPY -1.90008E+01
(CAL/G)
SP. HEAT (CP) 3.91666E-01
(CAL/G/DEG K)

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 0
AVERAGE STEP SIZE 0.00000E+00
METHOD ORDER 0
TOTAL NUMBER OF STEPS 0
FUNCT EVALUATIONS 0
JACOBIAN EVALUATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSIT- TIVE DIR RATE
CH3OH	2.04685E-06	2.18343E-01	-2.53107E-06	1	1.1375E+05	2.82759E+01	1.00000
CH3	0.00000E+00	0.00000E+00	2.18255E-06	2	1.1092E+05	4.51524E+01	1.00000
OH	0.00000E+00	0.00000E+00	2.18255E-06	3	1.8443E+12	0.00000E+00	0.00000
O2	1.53514E-06	1.63757E-01	-1.76032E-03	4	6.5683E+11	0.00000E+00	0.00000
CH2OH	0.00000E+00	0.00000E+00	3.48520E-07	5	2.1298E+12	0.00000E+00	0.00000
H02	0.00000E+00	0.00000E+00	3.48520E-07	6	6.4263E+11	0.00000E+00	0.00000
H20	0.00000E+00	0.00000E+00	0.00000E+00	7	4.5030E+09	0.00000E+00	0.00000
O	0.00000E+00	0.00000E+00	1.75997E-03	8	3.4507E+09	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	0.00000E+00	9	3.3312E+08	0.00000E+00	0.00000
H2	0.00000E+00	0.00000E+00	0.00000E+00	10	9.8019E+10	0.00000E+00	0.00000
CH4	0.00000E+00	0.00000E+00	0.00000E+00	11	3.2129E+02	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	12	1.2383E+12	0.00000E+00	0.00000
CH2O	0.00000E+00	0.00000E+00	0.00000E+00	13	3.0575E+04	0.00000E+00	0.00000
CH3O	0.00000E+00	0.00000E+00	0.00000E+00	14	2.0344E+12	0.00000E+00	0.00000
C2H6	0.00000E+00	0.00000E+00	0.00000E+00	15	3.5949E+12	0.00000E+00	0.00000
C2H5	0.00000E+00	0.00000E+00	0.00000E+00	16	3.6197E+08	0.00000E+00	0.00000
C2H4	0.00000E+00	0.00000E+00	0.00000E+00	17	6.3000E+12	0.00000E+00	0.00000
CH2	0.00000E+00	0.00000E+00	0.00000E+00	18	1.4742E+10	0.00000E+00	0.00000
C2H3	0.00000E+00	0.00000E+00	0.00000E+00	19	1.3634E+13	0.00000E+00	0.00000
C2H2	0.00000E+00	0.00000E+00	0.00000E+00	20	3.0893E+12	0.00000E+00	0.00000
HCO	0.00000E+00	0.00000E+00	1.45987E-03	21	5.4122E+12	0.00000E+00	0.00000
CH2O2	0.00000E+00	0.00000E+00	0.00000E+00	22	2.2721E+15	0.00000E+00	0.00000
C2H	0.00000E+00	0.00000E+00	0.00000E+00	23	6.1437E+11	0.00000E+00	0.00000
CO	0.00000E+00	0.00000E+00	8.38746E-07	24	2.8870E+11	0.00000E+00	0.00000
C2HO	0.00000E+00	0.00000E+00	0.00000E+00	25	4.8000E+13	0.00000E+00	0.00000

TABLE D.2.—Continued.

(j) Continued.

CH	9.37466E-11	1.00000E-05	-1.43990E-03	26	2.0000E+13	0.00000E+00	0.00000
CO2	2.19831E-09	2.34500E-04	-8.38746E-07	27	2.8928E+12	0.00000E+00	0.00000
H2	5.72199E-06	6.10380E-01	-3.43008E-08	28	1.2118E+04	0.00000E+00	0.00000
HCN	0.00000E+00	0.00000E+00	3.43008E-08	29	2.9817E+12	0.00000E+00	0.00000
N	9.37466E-12	1.00000E-06	-8.12589E-06	30	1.3792E+12	0.00000E+00	0.00000
CN	9.37466E-12	1.00000E-06	-3.12776E-04	31	2.1308E+12	0.00000E+00	0.00000
HNCO	0.00000E+00	0.00000E+00	0.00000E+00	32	3.6088E+12	0.00000E+00	0.00000
NCO	0.00000E+00	0.00000E+00	3.12776E-04	33	1.2515E+10	0.00000E+00	0.00000
NH2	0.00000E+00	0.00000E+00	0.00000E+00	34	4.3844E+12	0.00000E+00	0.00000
NO	0.00000E+00	0.00000E+00	8.16019E-06	35	6.0000E+12	0.00000E+00	0.00000
NH	0.00000E+00	0.00000E+00	0.00000E+00	36	3.3000E+13	0.00000E+00	0.00000
NO2	0.00000E+00	0.00000E+00	0.00000E+00	37	5.0000E+12	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	2.29236E-16	38	3.0000E+13	0.00000E+00	0.00000
HNO2	0.00000E+00	0.00000E+00	0.00000E+00	39	3.0000E+13	0.00000E+00	0.00000
HNO3	0.00000E+00	0.00000E+00	0.00000E+00	40	4.3144E-02	0.00000E+00	0.00000
HNO	0.00000E+00	0.00000E+00	0.00000E+00	41	3.4790E+12	0.00000E+00	0.00000
AR	6.82936E-08	7.28507E-03	0.00000E+00	42	6.4558E+12	0.00000E+00	0.00000
				43	4.1931E+11	0.00000E+00	0.00000
				44	2.9616E+11	0.00000E+00	0.00000
				45	2.7977E+13	0.00000E+00	0.00000
				46	2.0000E+13	0.00000E+00	0.00000
				47	5.5471E+11	0.00000E+00	0.00000
				48	1.2020E+12	0.00000E+00	0.00000
				49	1.0000E+13	0.00000E+00	0.00000
				50	5.0000E+13	0.00000E+00	0.00000
				51	3.0000E+13	0.00000E+00	0.00000
				52	4.6107E+12	0.00000E+00	0.00000
				53	1.0000E+13	0.00000E+00	0.00000
				54	2.8000E+13	0.00000E+00	0.00000
				55	2.3481E+12	0.00000E+00	0.00000
				56	2.9976E+12	0.00000E+00	0.00000
				57	3.3895E+12	0.00000E+00	0.00000
				58	2.2597E+12	0.00000E+00	0.00000
				59	2.0000E+13	0.00000E+00	0.00000
				60	1.6373E+06	0.00000E+00	0.00000
				61	5.0000E+13	0.00000E+00	0.00000
				62	6.2318E+11	0.00000E+00	0.00000
				63	2.0000E+13	0.00000E+00	0.00000
				64	1.2068E+03	0.00000E+00	0.00000
				65	1.8853E+13	0.00000E+00	0.00000
				66	5.3535E+12	0.00000E+00	0.00000
				67	8.9946E+12	0.00000E+00	0.00000
				68	5.5341E+10	0.00000E+00	0.00000
				69	1.0817E+13	0.00000E+00	0.00000
				70	2.0000E+13	0.00000E+00	0.00000
				71	7.7746E+00	0.00000E+00	0.00000
				72	1.5745E+09	0.00000E+00	0.00000
				73	1.1903E+09	0.00000E+00	0.00000
				74	1.5745E+09	0.00000E+00	0.00000
				75	3.7000E+12	9.87849E+00	1.00000
				76	1.0000E+13	1.86443E+04	1.00000
				77	1.2186E+12	0.00000E+00	0.00000
				78	1.3913E+09	0.00000E+00	0.00000
				79	1.8368E+12	0.00000E+00	0.00000
				80	7.0693E+12	0.00000E+00	0.00000
				81	5.0000E+12	0.00000E+00	0.00000
				82	4.0000E+13	0.00000E+00	0.00000
				83	3.0000E+13	0.00000E+00	0.00000
				84	3.0000E+13	0.00000E+00	0.00000
				85	3.0000E+13	0.00000E+00	0.00000
				86	2.0000E+13	0.00000E+00	0.00000
				87	6.9959E+11	0.00000E+00	0.00000
				88	4.9088E+14	-3.2620E-11	1.00000
				89	2.4017E+04	0.00000E+00	0.00000
				90	2.8315E+11	0.00000E+00	0.00000
				91	8.0313E+09	0.00000E+00	0.00000
				92	5.5600E+10	0.00000E+00	0.00000
				93	3.3065E+11	0.00000E+00	0.00000
				94	2.0496E+12	0.00000E+00	0.00000
				95	3.1968E+13	0.00000E+00	0.00000
				96	3.3951E+13	0.00000E+00	0.00000
				97	8.0000E+12	0.00000E+00	0.00000
				98	8.8557E+13	0.00000E+00	0.00000
				99	4.9579E+09	0.00000E+00	0.00000
				100	3.5069E+12	0.00000E+00	0.00000
				101	1.8000E+12	0.00000E+00	0.00000
				102	7.8000E+11	0.00000E+00	0.00000
				103	3.2169E+09	0.00000E+00	0.00000
				104	4.4731E+12	0.00000E+00	0.00000
				105	2.1501E+15	0.00000E+00	0.00000
				106	2.7435E-03	0.00000E+00	0.00000
				107	5.4615E+15	0.00000E+00	0.00000
				108	1.5972E-02	0.00000E+00	0.00000
				109	1.9970E-05	3.72320E-09	1.00000
				110	6.3946E+07	4.44383E-01	1.00000
				111	7.7115E+12	0.00000E+00	0.00000
				112	2.6452E+10	0.00000E+00	0.00000
				113	1.3531E+11	0.00000E+00	0.00000
				114	1.2000E+13	0.00000E+00	0.00000
				115	2.4505E+13	0.00000E+00	0.00000
				116	3.0688E+12	0.00000E+00	0.00000
				117	3.7241E+12	0.00000E+00	0.00000
				118	2.1729E+13	4.05117E+03	1.00000
				119	3.7000E+12	9.87849E-01	1.00000
				120	2.0000E+13	0.00000E+00	0.00000
				121	1.0000E+13	0.00000E+00	0.00000
				122	2.0000E+13	0.00000E+00	0.00000
				123	3.4124E+11	0.00000E+00	0.00000
				124	2.0000E+12	0.00000E+00	0.00000
				125	8.3121E+12	0.00000E+00	0.00000
				126	2.5138E+12	0.00000E+00	0.00000
				127	7.9397E+12	0.00000E+00	0.00000
				128	8.8054E+15	0.00000E+00	0.00000
				129	1.9643E+14	0.00000E+00	0.00000
				130	8.8159E+05	0.00000E+00	0.00000
				131	5.4802E+05	-1.05719E+02	1.00000
				132	2.7320E+01	0.00000E+00	0.00000
				133	4.0000E+12	0.00000E+00	0.00000
				134	1.3420E+05	0.00000E+00	0.00000
				135	1.9472E+09	-2.85326E-09	1.00000
				136	2.5078E+09	0.00000E+00	0.00000
				137	2.1964E+11	0.00000E+00	0.00000
				138	3.1979E+08	0.00000E+00	0.00000

TABLE D.2.—Continued.
(j) Continued.

				139	1.3060E+16	0.00000E+00	0.00000
				140	1.0814E+16	0.00000E+00	0.00000
				141	5.0000E+12	0.00000E+00	0.00000
				142	6.8118E+15	0.00000E+00	0.00000
				143	3.6000E+13	0.00000E+00	0.00000
DERIVATIVES (CGS UNITS): T							
	1.16420E+06	RHO	0.00000E+00				
MIXTURE MOLECULAR WEIGHT 29.63652 TOTAL ENERGY EXCHANGE RATE -1.37013E+09 MASS FRACTION SUM 1.00000000							
(CAL-CM**3/G**2/SEC)							
CPU TIME FOR INITIALIZATION OF LSENS = 2.320000 S							
TIME	6.50000E-04 SEC	AREA	0.00000E+00 SQ CM	AXIAL POSITION	0.00000E+00 CM		
FLOW PROPERTIES				INTEGRATION INDICATORS			
PRESSURE (ATM)	1.23771			STEPS FROM LAST PRINT	22		
VELOCITY (CM/SEC)	0.00			AVERAGE STEP SIZE	0.66459E-05		
DENSITY (G/CM**3)	2.77826E-04			METHOD ORDER	3		
TEMPERATURE (DEG K)	1558.04						
MASS FLOW RATE (G/SEC)	0.00000E+00			TOTAL NUMBER OF STEPS	169		
ENTROPY (CAL/G/DEG K)	2.2970			FUNCT EVALUATIONS	233		
MACH NUMBER	0.0000			JACOBIAN EVALUATIONS	31		
GAMMA	1.2057						
ENTHALPY (CAL/O)	1.71763E+00						
SP HLAT (CP) (CAL/G/DEG K)	4.05863E-01						
CHEMICAL PROPERTIES							
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
CH3OH	1.63313E-06	1.68690E-01	-6.53904E-03	1	1.9203E+07	3.85401E+03	0.97983
CH3	1.33680E-09	1.38082E-04	7.70793E-05	2	2.8986E+06	-1.76478E+03	0.95940
OH	1.32068E-09	1.36417E-04	3.77190E-05	3	2.0966E+12	5.85032E+04	0.99861
O2	1.21777E-06	1.25787E-01	-5.26103E-03	4	7.6119E+11	6.48800E+02	0.99745
CH2OH	2.74785E-08	2.83833E-03	6.17805E-04	5	3.3361E+12	1.11148E+04	0.99998
H2O	3.63008E-08	3.74961E-03	2.38526E-04	6	9.0266E+11	3.07071E+03	0.99768
H	5.47129E-07	5.65144E-02	1.01648E-02	7	8.4404E+09	2.38172E+02	0.99861
O	4.03882E-11	4.17181E-06	1.94849E-06	8	1.1969E+10	9.05141E+03	0.98463
H2	1.60786E-10	1.66080E-05	6.73690E-06	9	2.1382E+09	7.36906E+03	0.99999
CH4	3.49320E-08	3.60823E-03	9.63257E-04	10	1.4400E+11	6.24186E+04	0.99986
H2O2	1.40417E-09	1.45041E-04	5.52713E-05	11	9.0586E+04	-1.14317E+01	0.99861
CH2O	4.42219E-09	4.56781E-04	-1.59208E-04	12	2.6985E+12	-6.23307E+01	0.88760
CH3O	1.74995E-07	1.80757E-02	7.45257E-04	13	1.1081E+06	-2.60466E+02	0.99991
CH3O2	2.00942E-10	2.07559E-05	8.70415E-06	14	4.3128E+12	-3.15656E-01	0.99906
C2H6	1.73379E-10	1.79088E-05	1.34871E-05	15	4.9565E+12	4.75206E+01	0.80152
C2H5	1.56951E-13	1.62119E-08	1.21006E-08	16	2.2761E+09	3.84768E+01	0.98216
C2H4	1.00184E-10	1.03483E-05	7.00562E-06	17	6.3000E+12	-7.93508E+03	0.99999
CH2	1.87284E-14	1.93451E-09	2.00003E-09	18	5.6657E+10	1.42790E+03	0.88695
C2H3	8.18959E-14	8.45925E-09	8.04100E-09	19	5.7535E+12	2.60414E+02	0.99959
C2H2	7.69929E-13	7.95280E-08	7.80136E-08	20	8.9524E+12	2.07708E+00	0.99995
HCO	9.08209E-11	9.38114E-06	2.94632E-06	21	2.7910E+13	8.12125E-01	0.99997
C2H2O	1.46431E-11	1.51253E-06	4.90586E-07	22	4.4829E+12	8.50527E+01	0.96380
C2H	1.71430E-17	1.77075E-12	1.54283E-12	23	4.4829E+12	4.57667E-01	0.46462
CO	1.99746E-07	2.06323E-02	4.65676E-03	24	3.9780E+11	1.56860E-02	0.99955
C2HO	7.94533E-14	8.20695E-09	5.48424E-09	25	4.8000E+13	6.48297E-03	0.99936
CH	8.49693E-18	8.77672E-13	1.11920E-12	26	2.0000E+13	1.15756E+00	0.99708
CO2	1.01831E-08	1.05184E-03	3.35056E-04	27	5.5630E+12	2.45785E-02	0.99980
N2	5.72199E-06	5.91040E-01	-5.05261E-11	28	1.9560E+06	5.52929E+00	0.99980
HCN	2.01536E-14	2.08172E-09	9.90791E-11	29	3.2263E+12	-1.23202E+01	0.83051
N	5.89751E-16	6.09170E-11	-5.62587E-12	30	1.4668E+12	1.20085E+01	0.99995
CN	4.90811E-17	5.06972E-12	-2.58885E-12	31	2.2909E+12	2.60168E-01	0.99809
HNCO	8.91339E-12	9.20688E-07	-8.54386E-09	32	4.9725E+12	9.98414E-01	1.00000
HCO	6.72064E-15	6.94193E-10	-3.75436E-10	33	9.7365E+10	5.57482E+00	0.99998
NH2	2.54211E-13	2.62582E-08	8.79590E-09	34	4.3147E+12	1.02354E-03	1.00000
HO	2.43236E-12	2.51245E-07	6.19354E-08	35	6.0000E+12	1.41411E-03	1.00000
NH	6.89483E-14	7.12186E-09	-9.19723E-10	36	3.3000E+13	7.00620E-03	0.99194
H2O2	7.05138E-12	7.28356E-07	-6.09991E-08	37	5.0000E+12	5.91324E-07	0.99996
H2O	1.12947E-15	1.16666E-10	4.97219E-11	38	3.0000E+13	5.45639E-10	0.97550
HO2	3.80009E-16	3.92522E-11	1.62051E-12	39	3.0000E+13	-1.58106E-07	1.00000
H2O3	6.23374E-17	6.43900E-12	-1.52202E-12	40	4.1125E+01	2.64231E-03	0.99966
H2O	1.77972E-16	1.83832E-11	6.24962E-12	41	6.5588E+12	5.14950E-03	0.96582
AR	6.82936E-08	7.05423E-03	0.00000E+00	42	1.2787E+13	8.32266E-05	0.96732
				43	6.5680E+11	8.33024E-03	0.99998
				44	2.9998E+11	5.83425E-06	0.99453
				45	3.0801E+13	8.16209E-01	1.00000
				46	2.0000E+13	4.99717E-05	1.00000
				47	6.5114E+11	1.35703E-02	0.99822
				48	1.2020E+12	8.23793E-03	0.99549
				49	1.0000E+13	5.78345E-07	1.00000
				50	5.0000E+13	3.15611E-08	0.31254
				51	3.0000E+13	8.17857E-07	1.00000
				52	5.2415E+12	-7.63317E+00	0.52109
				53	1.0000E+13	7.08983E-01	0.99428
				54	2.8000E+13	9.72715E-02	0.85394
				55	2.8461E+12	1.58040E-01	0.91527
				56	3.7344E+12	2.86127E-02	0.98953
				57	5.6609E+12	1.55234E-01	1.00000
				58	3.7739E+12	1.36488E-01	0.96915
				59	2.0000E+13	4.48502E-07	1.00000
				60	7.6681E+07	3.12784E+03	0.99979
				61	5.0000E+13	8.37147E+00	1.00000
				62	9.8684E+11		
				63	2.0000E+13		

TABLE D.2.—Continued.
(j) Concluded.

64	2.1722E+05	4.73997E+00	0.99417
65	2.0361E+13	6.09633E+04	0.00000
66	6.8905E+12	2.51158E+03	0.99993
67	1.1265E+13	1.03143E+03	0.99999
68	5.6840E+10	1.72264E+02	0.99999
69	1.1842E+13	1.86258E+01	0.00000
70	2.0000E+13	1.25735E+04	0.99999
71	2.7611E+03	3.65187E-04	0.78882
72	9.2340E+09	2.56459E-02	0.99738
73	6.9937E+09	4.89074E-03	0.99968
74	9.2340E+09	2.11167E-01	0.99982
75	3.7000E+12	4.07506E-06	0.98251
76	1.0000E+13	1.34054E-03	0.00000
77	2.0845E+12	1.15853E-01	0.99999
78	8.2567E+09	8.06615E-08	0.99690
79	2.9355E+12	9.39004E-04	0.99830
80	1.1036E+13	4.19718E-04	0.97489
81	5.0000E+12	2.27048E-08	0.99929
82	4.0000E+13	1.81768E-07	0.00000
83	3.0000E+13	4.29504E+04	0.99918
84	5.0000E+13	1.42566E+00	0.00000
85	5.0000E+13	4.66185E+01	0.00000
86	2.0000E+13	3.78370E+00	0.00000
87	1.8983E+12	2.16223E+04	0.99994
88	6.3840E+14	6.45965E-01	0.00000
89	5.1092E+05	1.61000E+00	0.00000
90	3.0190E+11	1.03115E+05	0.99928
91	5.4932E+10	3.28146E+03	0.00000
92	1.8047E+11	4.28732E+01	0.45550
93	9.4625E+11	2.39177E+03	0.99660
94	4.9488E+12	7.92756E+01	0.87640
95	3.6636E+13	2.76799E+03	0.99930
96	3.6199E+13	6.87505E+02	0.99999
97	8.0000E+12	4.96858E+03	0.99930
98	9.4845E+13	7.17182E+03	0.00000
99	2.4624E+10	1.03391E+02	0.25735
100	5.8436E+12	2.64435E+02	0.90735
101	1.8000E+12	3.07104E+04	0.99999
102	7.8000E+11	7.18510E+00	0.00000
103	5.9507E+10	4.16562E+04	0.99999
104	6.6130E+12	3.68553E+03	0.99999
105	2.0166E+15	1.61735E+05	0.99999
106	2.3212E+00	4.64858E-01	0.99999
107	4.5570E+15	3.70595E-03	0.99999
108	7.5210E+00	6.61221E-03	0.99999
109	5.2192E-02	6.44117E-06	0.99999
110	2.1618E+08	1.36171E-07	0.99999
111	1.0832E+13	2.36344E-04	0.98999
112	8.8405E+10	5.57884E-06	0.85000
113	1.6192E+11	1.04156E-03	0.99999
114	1.2000E+13	3.08177E-07	0.00000
115	3.6000E+13	1.60391E-05	0.55000
116	5.4645E+12	4.30678E-03	0.25000
117	6.4222E+12	1.13958E-01	0.95566
118	2.3167E+13	1.79096E-02	0.99834
119	3.7000E+12	1.81346E-02	0.99838
120	2.0000E+13	7.03312E-05	0.00300
121	1.0000E+13	5.13490E-10	0.00000
122	2.0000E+13	2.78145E-04	0.99999
123	6.4538E+11	1.66249E-10	0.96306
124	2.0000E+12	5.35464E-10	0.99999
125	1.0345E+13	1.21936E-02	0.99998
126	2.4381E+12	2.46566E+00	0.88406
127	8.6899E+12	3.04082E-02	0.99911
128	8.1743E+15	6.86823E-02	0.99794
129	2.1584E+14	3.17031E+00	0.00000
130	2.1507E+07	2.96171E-04	0.99971
131	9.1747E+06	1.17350E-02	0.00000
132	3.6266E+03	1.02750E-05	0.54629
133	4.0000E+12	2.15000E-07	0.00000
134	5.5025E+06	3.41388E-06	0.49878
135	1.1732E+10	2.46454E-06	0.39719
136	1.1725E+10	1.52015E-09	0.99993
137	5.7827E+11	3.55854E-07	0.70719
138	2.0526E+09	1.54867E-03	0.49932
139	1.0237E+16	3.70324E-05	0.00171
140	9.6973E+15	3.50407E-03	0.62567
141	5.0000E+12	1.00000E-06	0.96918
142	6.5548E+15	1.00000E-04	0.59745
143	5.0000E+13	1.00000E-04	0.99792

DERIVATIVES (CGS UNITS): 1 4.95379E+06 RHO 0.0000E+00
MIXTURE MOLECULAR HEIGHT 28.69745 TOTAL ENERGY EXCHANGE RATE 1.75210E+09 0.0000E+00 0.00000001

(CAL-CMMS/GMW2/SEC)

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 1.650002E+00 S UP TO THIS TIME - 11.150002E+00 S

(LSNS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS - 169
TOTAL NO. OF DERIVATIVE EVALUATIONS - 233
TOTAL NO. OF JACOBIAN EVALUATIONS - 31
TOTAL CPU TIME - 11.150002 S

TOTAL CPU TIME (INCLUDING I/O) REQUIRED: 14.839996 S

(LSNS) READ DATA FOR NEXT CASE

TABLE D.2.—Continued.

(k) Case 11

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM

NASA LEWIS RESEARCH CENTER

LESENS PROPANE-AIR HELL-STIRRED REACTOR + ROCKET EXP; EMAX=10-4 CASE 11

REACTION NUMBER	REACTION	REACTION RATE VARIABLES A N	ACTIVATION ENERGY
1			
2	1*CH3 + 1*CSH8 = 1*CH25 + 1*CH3	5.00000E+15 0.0000	83500.00
3	1*CH3 + 1*CSH7 = 1*CH4 + 1*CH3	3.55000E+12 0.0000	10300.00
4	1*CH3 + 1*CH4 = 1*CH24 + 1*CH3	3.00000E+14 0.0000	33200.00
5	1*H + 1*CH4 = 1*CH3 + 1*H	2.00000E+17 0.0000	88000.00
6	1*CH4 + 1*O2 = 1*CH3 + 1*H2	1.26000E+14 0.0000	11900.00
7	1*O + 1*CH4 = 1*CH3 + 1*OH	7.94000E+13 0.0000	56000.00
8	1*OH + 1*CH4 = 1*CH3 + 1*H2O	1.90000E+14 0.0000	11720.00
9	1*CH3 + 1*O2 = 1*CH3O + 1*O	2.50000E+13 0.0000	5010.00
10	1*CH3 + 1*OH = 1*CH3O + 1*H	2.40000E+13 0.0000	28680.00
11	M + 1*CH3O = 1*CH2O + 1*H	6.30000E+12 0.0000	0.00
12	2*CH3 = 1*CH2H6 + 1*CH2	5.00000E+13 0.0000	21000.00
13	1*H + 1*CH2H6 = 1*CH2H5 + 1*H2	2.40000E+14 -0.4000	0.00
14	1*O + 1*CH2H6 = 1*CH2H5 + 1*OH	1.32000E+14 0.0000	9700.00
15	1*OH + 1*CH2H6 = 1*CH2H5 + 1*H2O	1.13000E+14 0.0000	7850.00
16	M + 1*CH2H5 = 1*CH2H4 + 1*H	8.70000E+13 0.0000	3520.00
17	1*CH2H5 + 1*O2 = 1*CH2H4 + 1*H2	1.00000E+17 0.0000	51000.00
18	1*H + 1*CH2H5 = 1*CH2H4 + 1*H2	2.00000E+12 0.0000	5000.00
19	1*CH3 + 1*CH2H5 = 1*CH2H4 + 1*H	4.80000E+13 0.0000	0.00
20	1*H + 1*CH2H4 = 1*CH2H3 + 1*H	2.00000E+13 0.0000	0.00
21	M + 1*CH2H4 = 1*CH2H2 + 1*CH2H3	1.50000E+14 0.0000	10200.00
22	1*CH2H4 + 1*OH = 1*CH2H3 + 1*H2	2.60000E+17 0.0000	79300.00
23	1*CH2H4 + 1*OH = 1*CH3 + 1*H2O	4.80000E+12 0.0000	1230.00
24	1*CH2H4 + 1*O = 1*CH3 + 1*HCO	2.00000E+12 0.0000	960.00
25	1*CH2H4 + 1*O = 1*CH2O + 1*CH2	3.30000E+12 0.0000	1150.00
26	M + 1*CH2H3 = 1*CH2H2 + 1*CH	2.50000E+13 0.0000	5000.00
27	1*CH2H3 + 1*O2 = 1*CH2H2 + 1*HCO	3.00000E+15 0.0000	32000.00
28	1*CH2H3 + 1*H = 1*CH2H2 + 1*H2	3.98000E+12 0.0000	-250.00
29	1*CH2H3 + 1*O = 1*CH2H2O + 1*H	6.00000E+12 0.0000	0.00
30	1*CH2H3 + 1*OH = 1*CH2H2 + 1*H2O	3.30000E+13 0.0000	0.00
31	1*CH2H3 + 1*CH2 = 1*CH2H2 + 1*CH3	5.00000E+12 0.0000	0.00
32	1*CH2H3 + 1*CH2H2 = 2*CH2H	3.00000E+13 0.0000	0.00
33	M + 1*CH2H2 = 1*CH2H + 1*H	4.20000E+16 0.0000	107000.00
34	1*CH2H2 + 1*O = 1*CH2 + 1*CO	1.60000E+14 0.0000	9890.00
35	1*CH2H2 + 1*O = 1*CH2H + 1*H	4.00000E+14 0.0000	10660.00
36	1*CH2H2 + 1*OH = 1*CH2H + 1*H2O	6.30000E+12 0.0000	7000.00
37	1*CH2H2 + 1*OH = 1*CH2H2O + 1*H	3.20000E+11 0.0000	200.00
38	1*CH2H + 1*O2 = 1*CH2H + 1*O	5.00000E+13 0.0000	1500.00
39	1*CH2H + 1*OH = 1*CH2H + 1*H	2.00000E+13 0.0000	0.00
40	1*CH2H + 1*O2 = 2*CO + 1*OH	1.46000E+12 0.0000	2500.00
41	1*CH2H + 1*O = 2*CO + 1*H	1.20200E+12 0.0000	0.00
42	1*CH2H + 1*OH = 2*HCO	1.00000E+13 0.0000	0.00
43	1*CH2H + 1*H = 1*CH2 + 1*CH	5.00000E+13 0.0000	0.00
44	1*CH2H + 1*CH2 = 1*CH2H3 + 1*CO	3.00000E+13 0.0000	0.00
45	1*CH2H + 1*CH2 = 1*CH2H + 1*CH2H	1.00000E+13 0.0000	2000.00
46	2*CH2H2O = 1*CH2H2 + 2*CO	1.00000E+13 0.0000	0.00
47	1*CH2H2O + 1*OH = 1*CH2H2 + 1*HCO	2.80000E+13 0.0000	0.00
48	1*CH2H2O + 1*OH = 1*CH2H2 + 1*H2O	7.50000E+12 0.0000	3000.00
49	1*CH2H2O + 1*H = 1*CH3 + 1*CO	1.13000E+13 0.0000	3428.00
50	1*CH2H2O + 1*H = 1*CH2H2 + 1*H2	7.50000E+13 0.0000	8000.00
51	1*CH2H2O + 1*O = 1*CH2H2 + 1*OH	5.00000E+13 0.0000	8000.00
52	1*CH2H2O + 1*O = 1*CH2H2 + 1*CO	2.00000E+13 0.0000	0.00
53	M + 1*CH2H2O = 1*CH2H2 + 1*CO	2.00000E+16 0.0000	60000.00
54	1*CH2H + 1*O = 1*CH2 + 1*CH	5.00000E+13 0.0000	0.00
55	1*CH3O + 1*O2 = 1*CH2O + 1*H2	1.00000E+13 0.0000	7170.00
56	1*CH3O + 1*H = 1*CH2O + 1*H2	2.00000E+13 0.0000	0.00
57	M + 1*CH2O = 1*HCO + 1*H	5.00000E+16 0.0000	81000.00
58	1*CH2O + 1*OH = 1*HCO + 1*H2O	3.00000E+13 0.0000	1200.00
59	1*CH2O + 1*H = 1*HCO + 1*H2	2.50000E+13 0.0000	3990.00
60	1*CH2O + 1*O = 1*HCO + 1*OH	3.50000E+13 0.0000	3510.00
61	1*CH3 + 1*CH2O = 1*CH4 + 1*HCO	1.00000E+10 0.5000	6000.00
62	1*CH3 + 1*HCO = 1*CH4 + 1*CO	3.00000E+11 0.5000	0.00
63	1*CH3 + 1*H2O2 = 1*CH3O + 1*OH	2.00000E+13 0.0000	0.00
64	M + 1*CH3 = 1*CH2 + 1*H	1.95000E+16 0.0000	91600.00
65	1*H + 1*CH3 = 1*H2 + 1*CH2	2.70000E+11 0.6700	25700.00
66	1*O + 1*CH3 = 1*OH + 1*CH2	1.90000E+11 0.6800	25700.00
67	1*OH + 1*CH3 = 1*H2O + 1*CH2	2.70000E+11 0.6700	25700.00
68	1*CH + 1*CO2 = 1*HCO + 1*CO	3.70000E+12 0.0000	0.00
69	1*CH + 1*O2 = 1*HCO + 1*O	1.00000E+13 0.0000	0.00
70	1*CH2 + 1*O2 = 1*CH2H2O + 1*O	5.00000E+11 0.5000	6960.00
71	1*CH2 + 1*O = 1*CH + 1*OH	2.00000E+11 0.7000	25800.00
72	1*CH2 + 1*OH = 1*CH + 1*H2O	5.00000E+11 0.5000	5900.00
73	1*CH2 + 1*H = 1*CH + 1*H2	3.20000E+11 0.7000	4970.00
74			
75	2*CH2 = 1*CH2H3 + 1*H	5.00000E+12 0.0000	0.00
76	1*HCO + 1*O = 1*CO + 1*H2	4.00000E+13 0.0000	0.00
77	1*HCO + 1*O = 1*CO + 1*H2O	3.00000E+13 0.0000	0.00
78	1*HCO + 1*OH = 1*CO + 1*H	3.00000E+13 0.0000	0.00
79	1*HCO + 1*H = 1*CO + 1*H2	3.00000E+13 0.0000	0.00
80	M + 1*HCO = 1*H + 1*CO	2.00000E+13 0.0000	0.00
81	1*CO + 1*O = 1*CO2 + 1*H	2.90000E+14 0.0000	15570.00
82	1*CO + 1*O2 = 1*CO2 + 1*O	2.40000E+15 0.0000	4100.00
83	1*CO + 1*OH = 1*CO2 + 1*H	2.50000E+12 0.0000	47690.00
84	1*CO + 1*H2O2 = 1*CO2 + 1*OH	4.17000E+11 0.0000	1000.00
85	1*O + 1*H2O = 2*OH	5.75000E+13 0.0000	22930.00
86	1*H + 1*O2 = 1*OH + 1*O	6.80000E+13 0.0000	18365.00
87	1*O + 1*H2 = 1*OH + 1*H	1.89000E+14 0.0000	16400.00
88	1*H + 1*H2O2 = 1*H2 + 1*OH	4.20000E+14 0.0000	13750.00
89	1*O + 1*H2O2 = 1*H2 + 1*O2	7.28000E+13 0.0000	2126.00
90	1*H2O2 + 1*OH = 1*H2O + 1*O2	5.00000E+13 0.0000	1000.00
91	1*H + 1*H2O2 = 2*OH	8.00000E+12 0.0000	0.00
92	1*H2 + 1*H2O2 = 1*H2O2 + 1*H	1.34000E+14 0.0000	1070.00
93	1*OH + 1*H2O2 = 1*H2O2 + 1*H2	7.91000E+13 0.0000	25000.00
94	1*OH + 2*H2O2 = 1*H2O2 + 1*H2O	6.10000E+12 0.0000	1430.00
95	1*H + 2*H2O2 = 1*H2O2 + 1*O2	1.80000E+12 0.0000	0.00
96	M + 1*H2O2 = 2*OH + 1*H2O	7.80000E+11 0.0000	0.00
97	1*H2 + 1*OH = 1*H2O + 1*H	1.44000E+17 0.0000	45510.00
98	1*H + 1*O2 = 1*H2O + 1*H	4.74000E+13 0.0000	6098.00
99	M + 1*H2O = 1*H2 + 1*OH	1.46000E+15 0.0000	-1000.00
100	1*H + 1*O = 1*OH + 1*H	1.30000E+15 0.0000	105140.00
101	1*H + 1*H2 = 2*H	7.10000E+18 -1.0000	0.00
102	M + 1*O2 = 2*O	2.20000E+14 0.0000	96000.00
103	1*CH + 1*H2 = 1*HCH + 1*H	1.80000E+18 -1.0000	118020.00
104	1*CN + 1*H2 = 1*HCN + 1*H	1.00000E+11 0.0000	19000.00
		6.00000E+13 0.0000	5300.00

TABLE D.2.—Continued
(k) Continued.

105	1X0	+	1XHCN	=	1XQH	+	1XCN	1.40000E+11	0.6800	16900.00
106	1XOH	+	1XHCN	=	1XHCN	+	1XH	4.00000E+11	0.0000	2800.00
107	1XCH	+	1X0	=	1XCO	+	1XH	1.20000E+13	0.0000	0.00
108	1XCH	+	1XQH	=	1XCO	+	1XH	2.50000E+14	0.0000	6000.00
109	1XH2	+	1XHCN	=	1XHCN	+	1XH	1.00000E+14	0.0000	9000.00
110	1XHCN	+	1X0	=	1XH2	+	1XCO	1.00000E+14	0.0000	8500.00
111	1XCH	+	1X02	=	1XCO	+	1X0	3.20000E+13	0.0000	1000.00
112	1XCH	+	1XCO2	=	1XCO	+	1XCO	5.70000E+12	0.0000	0.00
113	1X0	+	1XCO	=	1XNO	+	1XCO	2.00000E+13	0.0000	0.00
114	1XH	+	1XCO	=	1XN2	+	1XCO	1.00000E+13	0.0000	0.00
115	1XH	+	1XCO	=	1XNH	+	1XCO	2.00000E+13	0.0000	0.00
116	1XCH	+	1XNO	=	1XN	+	1XHCN	1.60000E+13	0.0000	9940.00
117	1XCH	+	1XNO	=	1X0	+	1XHCN	2.00000E+12	0.0000	0.00
118	1XNH	+	1XOH	=	1XN	+	1XN2O	5.00000E+11	0.5000	2000.00
119	1XNO2	+	1XNO	=	1XNO2	+	1XOH	2.09000E+12	0.0000	-477.00
120	1X0	+	1XNO2	=	1XNO	+	1X02	1.00000E+13	0.0000	596.00
121	1XNO	+	1X0	=	1XNO2	+	M	5.62000E+15	0.0000	-1160.00
122	1XNO2	+	1XH	=	1XNO	+	1XOH	3.47000E+14	0.0000	1470.00
123	1XNO	+	1XH	=	1XN	+	1XOH	2.65000E+14	0.0000	5040.00
124	1XNO	+	1X0	=	1XN	+	1X02	3.80000E+09	1.0000	41370.00
125	1X0	+	1XN2	=	1XNO	+	1XN	1.80000E+14	0.0000	76250.00
126	1XH	+	1XNO2	=	2XNO	+	M	4.00000E+12	0.0000	0.00
127	M	+	1XN2O	=	1XN2	+	1X0	6.92000E+13	2.5000	65000.00
128	1X0	+	1XN2O	=	1XN2	+	1X02	1.00000E+14	0.0000	28020.00
129	1X0	+	1XN2O	=	2XNO	+	M	6.92000E+13	0.0000	26630.00
130	1XN2O	+	1XH	=	1XN2	+	1XOH	7.59000E+13	0.0000	15100.00
131	1XNO2	+	1XN2	=	1XHHO2	+	1XH	2.40000E+13	0.0000	29000.00
132	1XOH	+	1XNO2	=	1XHHO3	+	M	5.00000E+15	0.0000	-3800.00
133	1XOH	+	1XNO	=	1XHHO2	+	M	5.60000E+15	0.0000	-1700.00
134	1XHHO	+	1XH	=	1XN2	+	1XNO	5.00000E+12	0.0000	0.00
135	1XH	+	1XNO	=	1XHHO	+	M	5.40000E+15	0.0000	-600.00
136	1XHHO	+	1XOH	=	1XN2O	+	1XNO	3.60000E+13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	, 96) = 2.30000	M(O2	, 96) = 0.78000	M(H2O	, 96) = 6.00000	M(H2O2	, 96) = 6.60000
M(O2	, 98) = 1.30000	M(N2	, 98) = 1.30000	M(H2O	, 98) = 21.30000	M(O2	, 98) = 7.00000
M(H2	, 99) = 4.00000	M(O2	, 99) = 1.50000	M(H2O	, 99) = 20.00000	M(N2	, 99) = 1.50000
M(O2	, 99) = 4.00000	M(H2	, 101) = 4.10000	M(O2	, 101) = 2.00000	M(H2O	, 101) = 15.00000
M(H2	, 101) = 2.00000	M(O2	, 132) = 0.70000	M(H2	, 132) = 1.40000		

*** INITIAL CONDITIONS ***

TIME 0.00000E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 2.00000E-01 CM

FLOW PROPERTIES

PRESSURE 5.00000
(ATM)
VELOCITY 0.00
(CM/SEC)
DENSITY 2.96325E-03
(G/CM**3)
TEMPERATURE 614.00
(DEG K)
MASS FLOW RATE 1.00000E+01
(G/SEC)
ENTROPY 1.7275
(CAL/G/DEG K)
MACH NUMBER 0.0000
GAMMA 1.2954
ENTHALPY 3.60515E+01
(CAL/G)
SP. HLAT (CP) 2.91858E-01
(CAL/G/DEG K)

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 0
AVERAGE STEP SIZE 0.00000E+00
METHOD ORDER 0
TOTAL NUMBER OF STEPS 0
FUNCT EVALUATIONS 0
JACOBIAN EVALUATIONS 0

HEAT LOSS(QDOT/MDOT) = -1.2180E+00 CAL/G

CHEMICAL PROPERTIES

SPECIES	MASS FRACTION	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS. UNITS	NET REACTION CONV RATE (MOLE*CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
C3H8	8.73262E-02	5.91318E-02	-5.57359E-20	1	9.4978E-15	6.34742E-15	1.00000
C2H5	0.00000E+00	0.00000E+00	5.57359E-20	2	7.6560E+08	0.00000E+00	0.00000
CH3	0.00000E+00	0.00000E+00	5.57359E-20	3	4.5685E+02	0.00000E+00	0.00000
CH4	0.00000E+00	0.00000E+00	0.00000E+00	4	9.5046E-15	0.00000E+00	0.00000
C3H7	0.00000E+00	0.00000E+00	0.00000E+00	5	7.3221E+09	0.00000E+00	0.00000
C2H4	0.00000E+00	0.00000E+00	0.00000E+00	6	9.2670E-07	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	0.00000E+00	7	1.2796E+10	0.00000E+00	0.00000
H2	0.00000E+00	0.00000E+00	0.00000E+00	8	4.1177E+11	0.00000E+00	0.00000
O2	2.11252E-01	1.97108E-01	-1.91172E-34	9	1.4850E+03	0.00000E+00	0.00000
HO2	0.00000E+00	0.00000E+00	0.00000E+00	10	6.3000E+12	0.00000E+00	0.00000
O	0.00000E+00	0.00000E+00	1.96753E-34	11	1.6755E+06	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	0.00000E+00	12	1.8405E+13	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	13	4.6549E+10	0.00000E+00	0.00000
CH3O	0.00000E+00	0.00000E+00	0.00000E+00	14	1.8152E+11	0.00000E+00	0.00000
CH2O	0.00000E+00	0.00000E+00	0.00000E+00	15	4.8595E+12	0.00000E+00	0.00000
C2H6	0.00000E+00	0.00000E+00	0.00000E+00	16	9.2412E+05	0.00000E+00	0.00000
CH2	0.00000E+00	0.00000E+00	0.00000E+00	17	3.3213E+10	0.00000E+00	0.00000
C2H3	0.00000E+00	0.00000E+00	0.00000E+00	18	4.8000E+13	0.00000E+00	0.00000
C2H2	0.00000E+00	0.00000E+00	0.00000E+00	19	2.0000E+13	0.00000E+00	0.00000
HCO	0.00000E+00	0.00000E+00	0.00000E+00	20	5.5112E+10	0.00000E+00	0.00000
C2H2O	0.00000E+00	0.00000E+00	0.00000E+00	21	1.5638E-11	0.00000E+00	0.00000
C2H	0.00000E+00	0.00000E+00	0.00000E+00	22	1.7516E+12	0.00000E+00	0.00000

TABLE D.2.—Continued.
(k) Continued.

CO	0.00000E+00	0.00000E+00	1.16036E-40	23	9.1059E+11	0.00000E+00	0.00000
C2H0	0.00000E+00	0.00000E+00	0.00000E+00	24	1.3071E+12	0.00000E+00	0.00000
CH	0.00000E+00	0.00000E+00	0.00000E+00	25	4.1516E+11	0.00000E+00	0.00000
CO2	4.16200E-04	2.82378E-04	-1.16036E-40	26	1.2215E+04	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	27	4.8851E+12	0.00000E+00	0.00000
N2	6.89289E-01	7.34705E-01	-1.85592E-34	28	6.0000E+12	0.00000E+00	0.00000
HCH	0.00000E+00	0.00000E+00	0.00000E+00	29	3.3000E+13	0.00000E+00	0.00000
N	0.00000E+00	0.00000E+00	0.00000E+00	30	5.0000E+12	0.00000E+00	0.00000
CH	0.00000E+00	0.00000E+00	0.00000E+00	31	3.0000E+13	0.00000E+00	0.00000
HHCO	0.00000E+00	0.00000E+00	0.00000E+00	32	3.0000E+13	0.00000E+00	0.00000
NCU	0.00000E+00	0.00000E+00	0.00000E+00	33	3.4452E-22	0.00000E+00	0.00000
NH2	0.00000E+00	0.00000E+00	0.00000E+00	34	4.8287E+10	0.00000E+00	0.00000
HO	0.00000E+00	0.00000E+00	0.00000E+00	35	6.4224E+10	0.00000E+00	0.00000
NH	0.00000E+00	0.00000E+00	0.00000E+00	36	2.0311E+10	0.00000E+00	0.00000
N02	0.00000E+00	0.00000E+00	0.00000E+00	37	2.7162E+11	0.00000E+00	0.00000
N2O	0.00000E+00	0.00000E+00	0.00000E+00	38	1.4624E+13	0.00000E+00	0.00000
HNO2	0.00000E+00	0.00000E+00	0.00000E+00	39	2.0000E+13	0.00000E+00	0.00000
HNO3	0.00000E+00	0.00000E+00	0.00000E+00	40	1.8814E+11	0.00000E+00	0.00000
HNO	0.00000E+00	0.00000E+00	0.00000E+00	41	1.2020E+12	0.00000E+00	0.00000
AR	1.17370E-02	8.77283E-03	0.00000E+00	42	1.0000E+13	0.00000E+00	0.00000
				43	5.0000E+13	0.00000E+00	0.00000
				44	3.0000E+13	0.00000E+00	0.00000
				45	1.9414E+12	0.00000E+00	0.00000
				46	1.0000E+13	0.00000E+00	0.00000
				47	2.8000E+13	0.00000E+00	0.00000
				48	6.4155E+11	0.00000E+00	0.00000
				49	6.8061E+11	0.00000E+00	0.00000
				50	1.0654E+11	0.00000E+00	0.00000
				51	7.1026E+10	0.00000E+00	0.00000
				52	2.0000E+13	0.00000E+00	0.00000
				53	8.7978E-06	0.00000E+00	0.00000
				54	5.0000E+13	0.00000E+00	0.00000
				55	2.8047E+10	0.00000E+00	0.00000
				56	2.0000E+13	0.00000E+00	0.00000
				57	7.3703E-13	0.00000E+00	0.00000
				58	1.1220E+13	0.00000E+00	0.00000
				59	9.5000E+11	0.00000E+00	0.00000
				60	1.9711E+12	0.00000E+00	0.00000
				61	1.8131E+09	0.00000E+00	0.00000
				62	7.4337E+12	0.00000E+00	0.00000
				63	2.0000E+13	0.00000E+00	0.00000
				64	4.8477E-17	0.00000E+00	0.00000
				65	1.4180E+04	0.00000E+00	0.00000
				66	1.0640E+04	0.00000E+00	0.00000
				67	1.4180E+04	0.00000E+00	0.00000
				68	3.7000E+12	0.00000E+00	0.00000
				69	1.0000E+13	0.00000E+00	0.00000
				70	4.1275E+10	0.00000E+00	0.00000
				71	1.1732E+04	0.00000E+00	0.00000
				72	9.8397E+10	0.00000E+00	0.00000
				73	4.8735E+11	0.00000E+00	0.00000
				74	5.0000E+12	0.00000E+00	0.00000
				75	4.0000E+13	0.00000E+00	0.00000
				76	5.0000E+13	0.00000E+00	0.00000
				77	3.0000E+13	0.00000E+00	0.00000
				78	3.0000E+13	0.00000E+00	0.00000
				79	2.0000E+13	0.00000E+00	0.00000
				80	8.5245E+08	0.00000E+00	0.00000
				81	8.5337E+13	1.32146E-35	1.00000
				82	2.6482E-05	0.00000E+00	0.00000
				83	1.8373E+11	0.00000E+00	0.00000
				84	3.9616E+05	0.00000E+00	0.00000
				85	1.9751E+07	0.00000E+00	0.00000
				86	2.7477E+08	0.00000E+00	0.00000
				87	5.3582E+09	0.00000E+00	0.00000
				88	1.2747E+13	0.00000E+00	0.00000
				89	2.2031E+13	0.00000E+00	0.00000
				90	8.0000E+12	0.00000E+00	0.00000
				91	5.5750E+13	0.00000E+00	0.00000
				92	9.9901E+04	0.00000E+00	0.00000
				93	1.8894E+12	0.00000E+00	0.00000
				94	1.8000E+12	0.00000E+00	0.00000
				95	7.8000E+11	0.00000E+00	0.00000
				96	9.1062E+00	0.00000E+00	0.00000
				97	3.2006E+11	0.00000E+00	0.00000
				98	3.3136E+15	0.00000E+00	0.00000
				99	4.8974E-23	0.00000E+00	0.00000
				100	1.1564E+16	0.00000E+00	0.00000
				101	1.4852E-20	0.00000E+00	0.00000
				102	2.8745E-27	6.35490E-31	1.00000
				103	1.7261E+04	0.00000E+00	0.00000
				104	7.7920E+11	0.00000E+00	0.00000
				105	1.0632E+07	0.00000E+00	0.00000
				106	6.0310E+10	0.00000E+00	0.00000
				107	1.2000E+13	0.00000E+00	0.00000
				108	1.8293E+12	0.00000E+00	0.00000
				109	6.2590E+10	0.00000E+00	0.00000
				110	9.4292E+10	0.00000E+00	0.00000
				111	1.4100E+13	0.00000E+00	0.00000
				112	3.7000E+12	0.00000E+00	0.00000
				113	2.0000E+13	0.00000E+00	0.00000
				114	1.0000E+13	0.00000E+00	0.00000
				115	2.0000E+13	0.00000E+00	0.00000
				116	4.6348E+09	0.00000E+00	0.00000
				117	2.0000E+12	0.00000E+00	0.00000
				118	2.4053E+12	0.00000E+00	0.00000
				119	3.0898E+12	0.00000E+00	0.00000
				120	6.1356E+12	0.00000E+00	0.00000
				121	1.4542E+16	0.00000E+00	0.00000
				122	1.0401E+14	0.00000E+00	0.00000
				123	2.9978E-04	0.00000E+00	0.00000
				124	4.3907E-03	0.00000E+00	0.00000
				125	1.3017E-13	0.00000E+00	0.00000
				126	4.0000E+12	0.00000E+00	0.00000
				127	5.4114E-07	0.00000E+00	0.00000
				128	1.0628E+04	-2.11359E-29	1.00000
				129	2.2978E+04	0.00000E+00	0.00000
				130	3.2025E+08	0.00000E+00	0.00000
				131	1.1424E+03	0.00000E+00	0.00000
				132	6.7563E+16	0.00000E+00	0.00000

TABLE D.2.—Continued.

(k) Continued.

			133	2.2558E+16	0.00000E+00	0.00000
			134	5.0000E+12	0.00000E+00	0.00000
			135	8.8300E+15	0.00000E+00	0.00000
			136	3.6000E+13	0.00000E+00	0.00000
MIXTURE MOLECULAR HEIGHT	29.85917	TOTAL ENERGY EXCHANGE RATE (CAL/CM**3/GM**2/SEC)	5.42968E-10	MASS FRACTION SUM	1.0000008	

CPU TIME FOR INITIALIZATION OF LSENS = 2.010002 S

EQUILIBRIUM CONDITIONS

TIME 0.00000E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 2.00000E-01 CM

FLOW PROPERTIES

PRESSURE 5.00000
(ATM)
VELOCITY 0.00
(CM/SEC)
DENSITY 7.12405E-04
(G/CM**3)
TEMPERATURE 2205.10
(DEG K)
MASS FLOW RATE 1.00000E+01
(G/SEC)
ENTROPY 2.3430
(CAL/G/DEG K)
MACH NUMBER 0.0000
GAMMA 1.2663
ENTHALPY 3.60518E+01
(CAL/G)
SP. HEAT (CP) 3.66532E-01
(CAL/G/DEG K)

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 0
AVERAGE STEP SIZE 0.00000E+00
METHOD ORDER 0
TOTAL NUMBER OF STEPS 0
FUNCT EVALUATIONS 0
JACOBIAN EVALUATIONS 0

HEAT LOSS(QDOT/MDOT) = 6.7375E+00 CAL/G

CHEMICAL PROPERTIES

SPECIES	MASS FRACTION	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE*CM**3/GM**2/SEC)	NET RATE/POSITIVE DIR RATE
C3H8	4.40962E-09	2.57807E-09	-1.88763E-06	1	2.6497E+07	3.71932E+00	1.00000
C2H5	2.90615E-09	2.57807E-09	-1.64737E-04	2	3.3836E+11	-4.57303E-10	0.11906
CH3	1.50347E-09	2.57807E-09	1.09630E-02	3	1.5369E+11	2.15727E+04	1.00000
CH4	1.60426E-09	2.57807E-09	4.94927E-08	4	3.7953E+08	-4.97462E-03	0.77164
C3H7	4.30883E-09	2.57807E-09	-1.09486E-02	5	8.3358E+12	-7.04647E-02	0.77165
C2H4	2.80536E-09	2.57807E-09	1.11153E-02	6	2.3366E+08	-4.25136E-09	0.77165
H	2.52153E-05	6.44928E-04	1.67780E-04	7	1.3097E+13	-2.18241E-02	0.99960
H2	4.89789E-03	6.26407E-02	-4.66564E-06	8	7.9688E+12	-4.63861E-04	0.77165
O2	1.73353E-06	1.39666E-06	6.34629E-09	9	3.4491E+10	-4.63861E-04	0.99960
HO2	3.30067E-09	2.57807E-09	2.22312E-08	10	6.3000E+12	-1.26755E+01	1.00000
O	9.10483E-07	1.46711E-06	7.32341E-08	11	4.1461E+11	1.60820E+00	1.00000
OH	1.37839E-04	2.08944E-04	1.86705E-04	12	1.1037E+13	-6.00128E+00	1.00000
H2O	9.86353E-02	1.41152E-01	-8.80070E-07	13	1.4428E+13	2.15546E-02	0.59721
CH3OH	3.10341E-09	2.57807E-09	-7.27513E-06	14	1.8839E+13	6.40254E-05	0.59721
CH2O	2.42160E-08	2.07920E-08	-8.53875E-07	15	3.8963E+13	1.88587E-02	0.59721
C2H6	3.00694E-09	2.57807E-09	-3.06632E-06	16	8.4636E+13	3.28232E+02	0.99982
CH2	1.40268E-09	2.57807E-09	1.09127E-06	17	6.3896E+11	3.46091E-06	0.99981
C2H3	2.70457E-09	2.57807E-09	-4.01556E-06	18	4.8000E+13	1.20056E-01	0.99982
C2H2	2.60378E-09	2.57807E-09	4.70061E-06	19	2.0000E+13	1.41827E-05	0.78609
HCO	8.92784E-08	7.93176E-08	3.54974E-07	20	1.4627E+13	-5.16927E-02	0.58553
C2H2O	4.20373E-09	2.57807E-09	1.40355E-07	21	3.5930E+09	1.39274E-02	0.99953
C2H	2.50299E-09	2.57807E-09	-7.14720E-07	22	3.6252E+12	-4.15075E-03	0.58553
CO	1.16640E-01	1.07355E-01	6.14452E-07	23	1.6065E+12	1.30202E-03	1.00000
C2HO	4.10293E-09	2.57807E-09	-2.43131E-07	24	2.5499E+12	1.45106E-05	1.00000
CH	1.30189E-09	2.57807E-09	-1.35362E-06	25	7.9870E+12	4.54482E-05	0.99992
CO2	7.86172E-02	4.60536E-02	-4.93828E-07	26	2.0210E+12	7.83700E+00	0.99972
H2O2	3.40146E-09	2.57807E-09	-7.97699E-06	27	4.2137E+12	2.28275E-05	1.00000
H2	6.89273E-01	6.34337E-01	-2.17771E-06	28	6.0000E+12	1.50054E-02	0.99972
HCH	8.56052E-08	8.16619E-08	2.17771E-06	29	3.3000E+13	1.87777E-04	0.99991
N	1.40067E-09	2.57807E-09	4.27903E-08	30	5.0000E+12	4.05122E-03	0.99972
CH	2.60177E-09	2.57807E-09	-2.34320E-06	31	3.0000E+13	2.99999E-07	1.00000
HNCO	4.02371E-08	2.41102E-08	1.53519E-06	32	3.0000E+13	3.00000E-07	1.00000
HCO	4.20171E-09	2.57807E-09	-1.39270E-06	33	1.0432E+06	-5.42732E-03	0.99926
HN2	2.19562E-08	3.5282E-08	-9.96718E-14	34	1.6746E+13	8.34364E-05	0.87554
HO	3.44264E-05	2.95785E-05	2.43727E-05	35	3.5118E+13	-5.71055E-04	0.74076
NH	1.20716E-08	2.07275E-08	2.57321E-09	36	1.2752E+12	-1.38619E+00	0.99926
HU2	4.60055E-09	2.57807E-09	1.37363E-04	37	5.0572E+11	1.67923E-04	0.94713
H2O	4.40128E-09	2.57807E-09	1.52331E-09	38	3.5506E+13	1.91801E-04	0.67772
HN02	4.70134E-09	2.57807E-09	-2.55091E-05	39	2.0000E+13	1.61628E-02	0.99713
HN03	6.30128E-09	2.57807E-09	-1.37720E-04	40	8.2523E+11	4.47065E-06	1.00000
HN0	3.10140E-09	2.57807E-09	1.47813E-06	41	1.2020E+12	6.84023E-06	1.00000
AR	1.17370E-02	7.57455E-03	0.00000E+00	42	1.0000E+13	8.10465E-03	1.00000
				43	5.0000E+13	1.21044E-01	0.96774
				44	3.0000E+13	2.69818E-07	0.89939
				45	6.3355E+12	6.09884E-08	0.96265
				46	1.0000E+13	9.99999E-08	1.00000
				47	2.8000E+13	2.26922E-08	0.99996
				48	3.7821E+12	-3.36226E-02	0.91645
				49	5.1680E+12	1.28386E-02	0.99306
				50	1.2083E+13	-3.31554E-01	0.91645
				51	8.0553E+12	-5.02823E-04	0.91645
				52	2.0000E+13	1.13810E-04	0.99996
				53	2.2613E+10	5.38408E-02	0.61382
				54	5.0000E+13	2.83649E-04	0.99688
				55	1.9470E+12	1.05480E-05	1.00000
				56	2.0000E+13	5.00317E-02	1.00000
				57	4.6878E+08	6.12826E-08	0.00000

TABLE D.2.—Continued.
(k) Continued.

58	2.2813E+13	-2.00079E-07	0.00000
59	1.0057E+13	-1.41921E-07	0.00000
60	1.5710E+13	-4.40742E-10	0.00000
61	1.1941E+11	7.43132E-09	0.77165
62	1.4088E+13	3.34447E-06	0.77164
63	2.0000E+13	-4.82236E-04	0.99959
64	1.6273E+07	-3.44902E-03	0.98203
65	1.3314E+11	-1.81995E-02	0.98203
66	1.0119E+11	-3.14655E-05	0.98203
67	1.3314E+11	-5.89629E-03	0.98203
68	3.7000E+12	6.60950E-01	1.00000
69	1.0000E+13	5.41746E-05	1.00000
70	4.7959E+12	2.59789E-05	0.99989
71	1.2144E+11	-2.25645E-05	0.97028
72	6.1084E+12	-1.61644E-01	0.97028
73	2.2541E+13	-1.84111E+00	0.97028
74	5.0000E+12	-1.05910E-07	0.67930
75	4.0000E+13	3.99655E-07	0.99914
76	3.0000E+13	-1.47829E-04	0.02872
77	3.0000E+13	-2.06588E-08	0.00000
78	3.0000E+13	-3.48865E-06	0.00000
79	2.0000E+13	-6.18997E-06	0.00000
80	8.3030E+12	8.49213E-04	0.00000
81	9.4158E+14	-3.51168E-05	0.00001
82	4.6917E+07	-2.36450E-09	0.00000
83	3.3191E+11	-1.01411E-02	0.00000
84	3.0694E+11	3.66970E-03	0.02871
85	1.0288E+12	2.34161E-04	0.00000
86	4.4775E+12	4.13785E-06	0.00000
87	1.8217E+13	2.22077E-04	0.00000
88	4.4815E+13	3.21879E-03	0.02871
89	3.9798E+13	6.50254E-06	0.02871
90	8.0000E+12	1.86154E-04	0.02871
91	1.0497E+14	7.53943E-01	0.02871
92	2.6327E+11	-6.23228E-02	0.49349
93	4.4015E+12	1.76041E-03	0.49349
94	1.8000E+12	-1.65168E-08	0.47852
95	7.8000E+11	9.91290E-04	0.50803
96	4.4444E+12	1.56525E+01	0.50803
97	1.1787E+13	-1.49093E-01	0.00000
98	1.8343E+15	-8.79791E-03	0.02872
99	4.9363E+04	2.50316E-04	0.00001
100	3.2198E+15	-6.06735E-07	0.00000
101	6.7260E+04	1.17654E-04	0.00000
102	1.6396E+03	1.88539E-11	0.00001
103	1.3088E+09	3.22042E-03	1.00000
104	1.7900E+13	4.28116E+00	0.98432
105	5.5550E+11	-6.28647E-03	0.98432
106	2.1113E+11	-2.67956E-09	0.00000
107	1.2000E+13	6.76986E-05	0.99136
108	6.3573E+13	2.38200E-02	0.46231
109	1.2823E+13	3.02489E+00	0.97084
110	1.4373E+13	-1.96390E-07	0.00000
111	2.5471E+13	6.57923E-05	0.46231
112	3.7000E+12	3.05544E-01	0.46231
113	2.0000E+13	1.10496E-04	0.97084
114	1.0000E+13	9.47097E-08	0.94710
115	2.0000E+13	4.85729E-02	0.97084
116	1.6556E+12	1.89949E-04	1.00000
117	2.0000E+12	2.29462E-04	1.00000
118	1.4875E+13	4.35028E-02	0.44882
119	2.3304E+12	-2.79051E-03	0.91257
120	8.7283E+12	4.54522E-05	0.91508
121	7.3233E+15	-1.42368E-01	0.91508
122	2.4811E+14	5.67949E-01	0.91508
123	2.6532E+09	3.41768E-02	0.44882
124	6.6525E+08	1.94941E-05	0.44882
125	4.9894E+06	3.13554E-03	0.44882
126	4.0000E+12	3.38369E-08	0.84592
127	1.0947E+09	-1.23741E-03	0.22565
128	1.6707E+11	-2.77063E-07	0.22565
129	1.5877E+11	-2.63297E-07	0.22565
130	2.4192E+12	-1.76353E-03	0.22565
131	3.2062E+10	-8.54691E-03	0.52316
132	7.1407E+15	-2.71359E+02	1.00000
133	8.2542E+15	-5.02538E+01	0.95950
134	5.0000E+12	-1.73611E-02	0.58124
135	6.1924E+15	-2.85459E+00	0.58124
136	3.6000E+13	-4.04976E-02	0.58124

MIXTURE MOLECULAR HEIGHT 25.78071 TOTAL ENERGY EXCHANGE RATE 5.63445E+08 MASS FRACTION SUM 1.00000027
(CAL-CH**3/G**2/SEC)

COMPUTATIONAL WORK REQUIRED FOR EQUILIBRIUM CALCULATION:
NO. OF ITERATIONS = 14 CPU TIME = 9.000397E-02 S

INITIAL ESTIMATES (SIGMAS) AT TEMPERATURE = 2205.10 K.

C3H8 1.00000E-10
C2H5 1.00000E-10
CH3 1.00000E-10
CH4 1.00000E-10
C3H7 1.00000E-10
C2H6 1.00000E-10
H 2.50159E-05
H2 2.42975E-03
O2 5.41748E-08
H2O 1.00000E-10
O 5.69073E-08
OH 8.10468E-06
H2O 5.47511E-03
CH3O 1.00000E-10
CH2O 8.06494E-10
C2H6 1.00000E-10
CH2 1.00000E-10
C2H3 1.00000E-10

TABLE D.2.—Continued.
(k) Continued.

C2H2	1.00000E-10
HCO	3.07663E-09
C2H2O	1.00000E-10
C2H	1.00000E-10
CO	4.16416E-03
C2HO	1.00000E-10
CH	1.00000E-10
CO2	1.78636E-03
H2O2	1.00000E-10
H2	2.46051E-02
HCN	3.16756E-09
H	1.00000E-10
CH	1.00000E-10
HNCO	9.35203E-10
HCO	1.00000E-10
HH2	1.37034E-09
HO	1.14731E-06
HH	8.03991E-10
HO2	1.00000E-10
H2O	1.00000E-10
HNHO2	1.00000E-10
HNHO3	1.00000E-10
HNHO	1.00000E-10
AK	2.93807E-04

HELLSTIRRED REACTOR CALCULATION... LSENS PROPANE-AIR WELL-STIRRED REACTOR + ROCKET EXP; EMAX=10-4 CASE 11

		INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE	ATM	5.00000	5.00000	1.00000
TEMP.	DEG K	614.000	2190.94	3.56831
ENTROPY	CAL/GM-K	1.72748	2.33746	1.35310
DENSITY	GM/CM**3	2.96325E-03	7.19404E-04	0.24278
ENTHALPY	CAL/GM	36.0515	29.3850	0.815084
SP. HEAT (CP)	CAL/GM-K	2.91858E-01	3.66534E-01	1.25586
MOL. WT. OF MIXT		29.8592	25.8669	
GAMMA		1.2954	1.2652	

SPECIES	MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
C3H8	5.91318E-02	8.73262E-02	1.01503E-07	1.72695E-07
C2H5	0.00000E+00	0.00000E+00	2.52669E-09	2.90615E-09
CH3	0.00000E+00	0.00000E+00	2.71015E-04	1.58688E-04
CH4	0.00000E+00	0.00000E+00	9.45262E-04	5.86249E-04
C3H7	0.00000E+00	0.00000E+00	2.52669E-09	4.30883E-09
C2H4	0.00000E+00	0.00000E+00	8.88892E-06	9.64034E-06
H	0.00000E+00	0.00000E+00	7.91521E-04	3.08436E-05
H2	0.00000E+00	0.00000E+00	5.90258E-02	4.59986E-03
O2	1.97108E-01	2.11232E-01	8.06592E-05	9.95524E-05
HO2	0.00000E+00	0.00000E+00	7.60364E-08	9.70239E-08
O	0.00000E+00	0.00000E+00	2.62396E-06	1.62299E-06
OH	0.00000E+00	0.00000E+00	2.68915E-04	1.76810E-04
H2O	0.00000E+00	0.00000E+00	1.42406E-01	9.91795E-02
CH3O	0.00000E+00	0.00000E+00	1.05584E-07	1.23076E-07
CH2O	0.00000E+00	0.00000E+00	5.73864E-06	6.66138E-06
C2H6	0.00000E+00	0.00000E+00	7.57872E-07	8.81000E-07
CH2	0.00000E+00	0.00000E+00	6.74332E-06	3.65940E-06
C2H3	0.00000E+00	0.00000E+00	2.65585E-07	2.81870E-07
C2H2	0.00000E+00	0.00000E+00	5.91869E-04	5.95779E-04
HCO	0.00000E+00	0.00000E+00	1.15555E-07	1.29633E-07
C2H2O	0.00000E+00	0.00000E+00	4.41671E-06	7.17776E-06
C2H	0.00000E+00	0.00000E+00	5.43188E-07	5.25902E-07
CO	0.00000E+00	0.00000E+00	1.03564E-01	1.32470E-01
C2HO	0.00000E+00	0.00000E+00	8.02487E-07	1.27552E-06
CH	0.00000E+00	0.00000E+00	1.93182E-07	9.72290E-08
CO2	2.82378E-04	4.16200E-04	4.76000E-02	8.09863E-02
H2O2	0.00000E+00	0.00000E+00	2.58669E-09	5.40146E-09
H2	7.34705E-01	6.89289E-01	6.36424E-01	6.89235E-01
HCN	0.00000E+00	0.00000E+00	9.35685E-06	9.77598E-06
H	0.00000E+00	0.00000E+00	2.99478E-08	1.62165E-08
CH	0.00000E+00	0.00000E+00	2.58669E-09	2.60177E-09
HNCO	0.00000E+00	0.00000E+00	2.61621E-06	4.35160E-06
HO	0.00000E+00	0.00000E+00	1.04164E-08	1.69200E-08
HH2	0.00000E+00	0.00000E+00	4.95708E-06	3.07051E-06
HO	0.00000E+00	0.00000E+00	8.14463E-05	9.44791E-05
HH	0.00000E+00	0.00000E+00	1.38717E-07	8.05189E-08
HO2	0.00000E+00	0.00000E+00	2.58669E-09	4.60055E-09
H2O	0.00000E+00	0.00000E+00	2.58669E-09	4.40128E-09
HNHO2	0.00000E+00	0.00000E+00	2.58669E-09	4.70136E-09
HNHO3	0.00000E+00	0.00000E+00	2.58669E-09	6.50128E-09
HNHO	0.00000E+00	0.00000E+00	2.21709E-08	2.65825E-08
AK	8.77283E-03	1.17370E-02	7.59768E-03	1.17370E-02

HEAT LOSS(QDOT/MDOT) = 6.6668E+00 CAL/GM
VOLUME 300.000 CM**3 MASS FLO 10.0000 GM/SEC
MDOT/VOLUME = 0.03333 RESIDENCE TIME = 21.5821 MSEC ITERATIONS = 12

TABLE D.2.—Continued.
(k) Continued.

HELLSTIRRED REACTOR CALCULATION.... LSENS			PROPANE-AIR HELL-STIRRED REACTOR + ROCKET EXP; EMAX=10-4			CASE 11
INITIAL STATE			FINAL STATE	FINAL/INITIAL RATIO		
PRESSURE	ATM	5.00000	5.00000	1.00000		
TEMP.	DEG K	614.000	2148.67	3.49947		
ENTROPY	CAL/GM/K	1.72748	2.35082	1.34926		
DENSITY	GM/CM**3	2.96325E-03	7.36115E-04	0.24841		
ENTHALPY	CAL/GM	36.0515	36.0111	0.998881		
SP. HEAT (CP)	CAL/GM/K	2.91858E-01	3.66061E-01	1.25424		
MOL. HT. OF MIXT		29.8592	25.9571			
GAMMA		1.2954	1.2644			
SPECIES			MOLE FRACT	MASS FRACT	MOLE FRACT	MASS FRACT
C3H8		5.91318E-02	8.73262E-02	2.31540E-05	3.93342E-05	
C2H5		0.00000E+00	0.00000E+00	7.64447E-07	8.55872E-07	
CH3		0.00000E+00	0.00000E+00	1.75760E-03	1.00644E-03	
CH4		0.00000E+00	0.00000E+00	1.21288E-03	7.49611E-04	
C3H7		0.00000E+00	0.00000E+00	2.59571E-09	4.30883E-09	
C2H4		0.00000E+00	0.00000E+00	3.05887E-04	3.30592E-04	
H		0.00000E+00	0.00000E+00	4.66244E-05	1.81053E-04	
H2		0.00000E+00	0.00000E+00	4.75052E-02	3.67367E-03	
O2		1.97108E-01	2.11252E-01	2.19454E-03	2.70553E-03	
H2O		0.00000E+00	0.00000E+00	3.15354E-06	4.00975E-06	
O		0.00000E+00	0.00000E+00	1.52471E-04	9.39801E-05	
OH		0.00000E+00	0.00000E+00	1.93598E-03	1.26847E-03	
H2O		0.00000E+00	0.00000E+00	1.46084E-01	1.01388E-01	
CH3O		0.00000E+00	0.00000E+00	8.13630E-07	9.72770E-07	
CH2O		0.00000E+00	0.00000E+00	6.71907E-05	7.77237E-05	
C2H6		0.00000E+00	0.00000E+00	3.17376E-05	3.67656E-05	
CH2		0.00000E+00	0.00000E+00	1.73502E-04	9.38117E-05	
C2H3		0.00000E+00	0.00000E+00	1.95693E-05	2.03900E-05	
C2H2		0.00000E+00	0.00000E+00	2.66249E-03	2.67077E-03	
HCO		0.00000E+00	0.00000E+00	2.80311E-06	3.13369E-06	
C2H2O		0.00000E+00	0.00000E+00	4.49156E-05	7.27403E-05	
C2H		0.00000E+00	0.00000E+00	1.26075E-05	1.21572E-05	
CO		0.00000E+00	0.00000E+00	9.93922E-02	1.07254E-01	
C2HO		0.00000E+00	0.00000E+00	5.26326E-05	8.31942E-05	
CH		0.00000E+00	0.00000E+00	3.38357E-05	1.69704E-05	
CO2		2.82378E-04	4.16200E-04	4.54745E-02	7.71012E-02	
H2O2		0.00000E+00	0.00000E+00	1.48198E-07	1.94201E-07	
H2		7.34705E-01	6.89289E-01	6.38598E-01	6.89187E-01	
HCH		0.00000E+00	0.00000E+00	2.82088E-05	2.93700E-05	
H		0.00000E+00	0.00000E+00	3.93803E-07	2.12500E-07	
CH		0.00000E+00	0.00000E+00	9.97618E-08	9.99946E-08	
HHC0		0.00000E+00	0.00000E+00	4.02982E-06	6.67960E-06	
HCO		0.00000E+00	0.00000E+00	1.23855E-07	2.00486E-07	
H2		0.00000E+00	0.00000E+00	4.75288E-05	2.93380E-05	
H0		0.00000E+00	0.00000E+00	1.07732E-04	1.24536E-04	
H0		0.00000E+00	0.00000E+00	5.63310E-07	3.25840E-07	
H02		0.00000E+00	0.00000E+00	2.59571E-09	4.60055E-09	
H2O		0.00000E+00	0.00000E+00	3.33234E-08	5.65030E-08	
H0H02		0.00000E+00	0.00000E+00	2.59571E-09	4.70134E-09	
H0H03		0.00000E+00	0.00000E+00	2.59571E-09	6.30128E-09	
H0H0		0.00000E+00	0.00000E+00	1.79560E-07	2.14542E-07	
AR		8.77283E-03	1.17370E-02	7.62638E-03	1.17370E-02	

HEAT LOSS(QDOT/MDOT) = 4.0346E-02 CAL/GM

VOLUME 300.000 CM**3 MASS FLO 1600.00 GM/SEC
MDOT/VOLUME = 5.33333 RESIDENCE TIME = 0.1380 MSEC ITERATIONS = 4

COMPUTATIONAL WORK REQUIRED FOR PSR CALCULATION;
NO. OF ITERATIONS = 22 CPU TIME = 4.480003E+00 S

** INITIAL CONDITIONS **

TIME	0.00000E+00	SEC	AREA	1.90000E+01	SQ CM	AXIAL POSITION	2.00000E-01	CM
FLOW PROPERTIES						INTEGRATION INDICATORS		
PRESSURE (ATM)	5.00000		STEPS FROM LAST PRINT			0		
VELOCITY (CM/SEC)	114398.68		AVERAGE STEP SIZE			0.00000E+00		
DENSITY (G/CM**3)	7.36114E-04		METHOD ORDER			0		
TEMPERATURE (DEG K)	2148.67		TOTAL NUMBER OF STEPS			0		
MASS FLOW RATE (G/SEC)	1.60000E+03		FUNCT EVALUATIONS			0		
ENTROPY (CAL/G/DEG K)	2.3308		JACOBIAN EVALUATIONS			0		
MACH NUMBER	1.2263							
GAMMA	1.2644							
ENTHALPY (CAL/G)	3.60111E+01							
SP. HEAT (CP) (CAL/G/DEG K)	3.66061E-01							

TABLE D.2.—Continued.

(k) Continued.

CHAMBER PRESS = 73.5 PSIA THROAT AREA = 2.32500E+00 SQ IN

ISP = 1144.0 METERS/SEC = 116.7 LB-SEC/LB IVAC = 1745.6 METERS/SEC = 178.0 LB-SEC/LB

CSTAR = 1558.7 FT/SEC THRUST COEFF = 2.4079 AREA RATIO = 1.267

HEAT LOSS(QDDT/MDOT) = 4.0346E-02 CAL/(G-CM)

CHEMICAL PROPERTIES

SPECIES	MASS FRACTION	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE/CM**3/G**2/SEC)	NET RATE/POSITIONAL DIR RATE
C5H8	5.93342E-05	2.31540E-05	-1.05572E-02	1	1.6065E+07	1.94640E+04	0.99986
C2H5	8.55872E-07	7.64447E-07	1.57005E-07	2	3.1811E+11	1.8934E+01	0.99991
CH3	1.00644E-03	1.73760E-03	9.49976E-03	3	1.2596E+11	1.68917E+04	0.98718
CH4	7.49611E-04	1.21288E-03	2.49208E-04	4	2.2398E+08	-3.43897E+04	0.98841
C3H7	4.30883E-09	2.59571E-09	-9.14273E-03	5	7.7621E+12	2.28150E+04	0.99021
C2H4	3.30592E-04	3.05887E-04	9.20558E-03	6	1.5990E+08	-3.71835E+00	0.85479
H	1.81053E-04	4.66244E-03	9.59796E-04	7	1.2209E+13	1.47023E+03	0.43876
H2	5.67367E-03	4.73052E-02	9.71962E-03	8	7.7331E+12	9.78723E+03	0.36316
O2	2.70533E-03	2.19454E-03	-3.47558E-02	9	2.9044E+10	1.49213E+02	0.90775
H2O	4.00975E-06	3.15334E-06	6.36669E-07	10	6.3000E+12	2.48595E+02	0.00790
O	9.39801E-05	1.52471E-04	3.12865E-05	11	3.6558E+11	4.41374E+02	0.99980
OH	1.26847E-03	1.93598E-03	4.93335E-04	12	1.1152E+13	6.60346E+03	0.13214
H2O	1.01588E-01	1.46084E-01	3.00154E-02	13	1.3613E+13	2.98679E+03	0.99903
CH3O	9.72770E-07	8.13630E-07	1.66997E-07	14	1.7973E+13	1.28977E+02	0.99917
CH2O	7.77237E-05	6.71907E-05	1.38072E-05	15	3.8149E+13	5.47566E+03	0.99905
C2H6	3.67656E-05	3.17376E-05	6.51821E-06	16	7.0287E+13	2.58011E+04	0.99905
CH2	9.38117E-05	1.73602E-04	3.56721E-05	17	6.2010E+11	1.46062E+00	0.94602
C2H3	2.03900E-05	1.95693E-05	4.02397E-06	18	4.8000E+13	2.52622E+02	0.99491
C2H2	2.67077E-03	2.66249E-03	5.47053E-07	19	2.0000E+13	8.94556E+03	0.99905
HCO	3.13369E-06	2.80311E-06	5.80057E-07	20	1.3760E+13	2.86697E+04	0.98455
C2H2O	7.27403E-05	4.49156E-05	9.22834E-06	21	2.2339E+09	1.00839E+03	0.99428
C2H	1.21572E-05	1.26075E-05	2.58966E-06	22	3.5986E+12	3.11438E+03	0.98467
CO	1.07254E-01	9.93922E-02	2.58966E-06	23	1.5973E+12	1.40013E+03	0.99732
C2HO	8.31942E-05	5.26326E-05	1.08105E-05	24	2.5327E+12	1.75312E+02	1.00000
CH	1.69704E-05	3.38357E-05	6.95098E-06	25	7.7512E+12	5.55807E+02	0.98862
CO2	7.71012E-02	4.54745E-02	9.29308E-03	26	1.6683E+12	3.07399E+04	0.63639
H2O2	1.94201E-07	1.48198E-07	3.04412E-08	27	4.2200E+12	2.68978E+02	1.00000
H2	6.89187E-01	6.38598E-01	-1.94100E-05	28	6.0000E+12	8.10270E+02	0.99725
HCH	2.93700E-05	2.82088E-05	5.79600E-06	29	3.3000E+13	1.46137E+02	0.99999
N	9.99966E-08	9.97618E-08	8.09213E-08	30	5.0000E+12	2.80389E+02	0.99730
CH	6.67960E-06	4.02982E-06	8.27995E-07	31	3.0000E+13	1.50564E+02	0.99537
HCO	2.00486E-07	1.23855E-07	2.54486E-08	32	3.0000E+13	1.09451E+01	0.99634
H2	2.93380E-05	4.75288E-05	9.76560E-06	33	5.4938E+05	-2.14891E+02	0.99000
HO	1.24536E-04	1.07732E-04	2.62632E-06	34	1.5782E+13	5.08850E+03	0.99995
HH	3.25840E-07	5.63310E-07	1.15742E-07	35	3.2945E+13	1.97593E+04	0.99544
H2O	4.60055E-09	2.59571E-09	1.16773E-04	36	1.2228E+12	2.45186E+03	0.26210
H2O	5.65030E-08	3.33234E-08	6.84688E-09	37	3.0536E+11	2.32732E+03	0.99626
HHO2	4.70134E-09	2.59571E-09	1.77305E-05	38	3.5188E+13	1.44403E+03	0.99935
HHO3	6.30128E-09	2.59571E-09	-1.14993E-04	39	2.0000E+13	7.19438E+02	0.99299
HHO	2.14542E-07	1.79560E-07	3.68919E-08	40	8.1296E+11	1.39365E+02	1.00000
AR	1.17370E-02	7.62638E-03	0.00000E+00	41	1.2020E+12	1.43164E+01	1.00000
				42	1.0000E+13	1.51232E+03	1.00000
				43	5.0000E+13	1.79997E+04	1.00000
				44	3.0000E+13	4.06834E+02	0.98862
				45	6.2600E+12	8.48614E+01	1.00000
				46	1.0000E+13	4.11146E+01	0.99963
				47	2.8000E+13	5.61354E+03	1.00000
				48	3.7147E+12	-1.82554E+02	0.99997
				49	5.0629E+12	1.53042E+03	0.27578
				50	1.1517E+13	-1.46366E+03	0.97254
				51	7.6782E+12	-1.69263E+01	0.29021
				52	2.0000E+13	2.03284E+02	0.17823
				53	1.5783E+10	-1.22768E+03	1.00000
				54	5.0000E+13	1.42644E+02	0.99995
				55	1.8651E+12	4.94269E+00	0.99998
				56	2.0000E+13	1.12605E+02	1.00000
				57	2.8851E+08	2.47993E+01	0.86196
				58	2.2650E+13	4.36838E+03	0.99898
				59	9.8198E+12	4.56100E+03	0.99856
				60	5.5385E+13	2.35694E+02	0.99910
				61	1.1371E+11	1.96725E+01	0.99840
				62	1.3906E+13	1.00282E+07	0.99736
				63	2.0000E+13	1.61422E+02	0.99248
				64	9.3984E+06	-1.88849E+03	0.98733
				65	1.1217E+11	5.47249E+02	0.40575
				66	8.5229E+10	1.63117E+01	0.48673
				67	1.1217E+11	2.53868E+02	0.41760
				68	3.7000E+12	8.44952E+03	1.00000
				69	1.0000E+13	1.10206E+03	1.00000
				70	4.5407E+12	2.56751E+03	1.00000
				71	1.0217E+11	1.68649E+00	0.42016
				72	5.8205E+12	9.93108E+02	0.36207
				73	2.1486E+13	8.48369E+03	0.32868
				74	5.0000E+12	2.23643E+02	0.99997
				75	4.0000E+13	1.78919E+03	1.00000
				76	3.0000E+13	2.69292E+02	0.98313
				77	3.0000E+13	1.90039E+01	0.99863
				78	3.0000E+13	2.41254E+02	0.99844
				79	2.0000E+13	3.87330E+02	0.99841
				80	7.5634E+12	2.48318E+04	0.78916
				81	9.1872E+14	5.83201E+02	0.99521
				82	5.5254E+07	1.06319E+01	0.93158
				83	5.2993E+11	2.48913E+04	0.26417
				84	2.6755E+11	1.23752E+02	0.99462
				85	9.2158E+11	3.61643E+03	0.11870
				86	4.0584E+12	5.59004E+04	0.90702
				87	1.6776E+13	2.44723E+04	0.13627
				88	4.4247E+13	8.74413E+02	0.90564
				89	3.9560E+13	2.59288E+01	0.91850
				90	8.0000E+12	6.57821E+01	0.90752
				91	1.0430E+14	2.25860E+03	0.99242
				92	2.6644E+11	-2.76187E+01	0.00547
				93	4.3639E+12	4.70124E-02	0.02530
				94	1.8000E+12	2.40942E-02	0.80512
				95	7.8000E+11	7.93997E-01	0.99261

TABLE D.2.—Continued.
(k) Continued.

	96	3.3835E+12	-1.14933E+00	0.00086								
	97	1.1364E+13	3.07904E+04	0.01993								
	98	1.8453E+15	3.23997E+03	0.92020								
	99	2.6288E+04	-3.35336E+03	0.99262								
	100	5.5044E+15	9.82273E+01	0.99350								
	101	3.7836E+04	-1.34185E+03	0.99247								
	102	8.2955E+02	-3.59256E-02	0.93005								
	103	1.1680E+09	3.74563E+01	0.99999								
	104	1.7341E+13	-2.57872E+01	0.17513								
	105	4.9322E+11	9.05306E-01	0.28754								
	106	2.0762E+11	1.08876E+01	0.64699								
	107	1.2000E+13	2.70856E-01	0.99981								
	108	6.1328E+13	9.38431E+00	0.53382								
	109	1.2150E+13	8.66268E+00	0.08199								
	110	1.3659E+13	1.80222E+01	0.04731								
	111	2.5318E+13	7.87019E+00	0.95665								
	112	3.7000E+12	9.12932E+00	0.36645								
	113	2.0000E+13	5.60551E-01	0.99999								
	114	1.0000E+13	7.23902E-04	1.00000								
	115	2.0000E+13	1.71129E+01	0.99834								
	116	1.5599E+12	8.43899E+00	1.00000								
	117	2.0000E+12	1.08202E+01	1.00000								
	118	1.4509E+13	1.68993E+01	0.71962								
	119	2.3370E+12	1.15078E+00	0.97662								
	120	8.6972E+12	-1.26993E-02	0.71312								
	121	7.3744E+15	4.99607E+00	0.97993								
	122	2.4593E+14	-2.98561E+00	0.67588								
	123	1.9614E+09	-5.60612E+01	0.97458								
	124	5.0589E+08	-5.20566E+00	0.99764								
	125	3.1593E+06	-1.64848E+00	0.78311								
	126	4.0000E+12	6.01853E-06	0.99176								
	127	7.9120E+08	-4.79388E-01	0.92453								
	128	1.4125E+11	7.78928E-05	0.07313								
	129	1.3535E+11	1.01038E-03	0.98990								
	130	2.2099E+12	4.65644E-01	0.91382								
	131	2.6947E+10	-1.11662E-01	0.95787								
	132	7.3052E+15	-2.12217E+02	0.99999								
	133	8.3388E+15	3.28330E+01	0.44853								
	134	5.0000E+12	6.15514E+00	0.99073								
	135	6.2147E+15	2.46284E+01	0.18745								
	136	3.6000E+13	1.84052E+01	0.99092								
DERIVATIVES (CGS UNITS): T					-1.61242E+03	RHO	-2.23801E-03	V	2.27387E+05			
MIXTURE MOLECULAR WEIGHT					25.95711	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)		-4.71633E+09	MASS FRACTION SUM	1.00000018		
CPU TIME FOR INITIALIZATION OF LSENS =					0.599998 S							
TIME					2.10833E-05	SEC	AREA	9.50000E+01	SQ CM	AXIAL POSITION	4.00000E+00	CM
FLOW PROPERTIES							INTEGRATION INDICATORS					
PRESSURE							0.31213	STEPS FROM LAST PRINT			16	
VELOCITY (CM/SEC)							205745.31	AVERAGE STEP SIZE			0.13189E+00	
DENSITY (G/CM**3)							8.18530E-05	METHOD ORDER			4	
TEMPERATURE (DEG K)							1207.44					
MASS FLOW RATE (G/SEC)							1.59988E+03	TOTAL NUMBER OF STEPS			158	
ENTROPY (CAL/G/DEG K)							2.3367	FUNCI EVALUATIONS			203	
MACH NUMBER							2.9058	JACOBIAN EVALUATIONS			30	
GAMMA							1.2975					
ENTHALPY (CAL/G)							-3.13534E+02					
SP. HEAT (CP) (CAL/G/DEG K)							3.53538E-01					
CHAMBER PRESS = 75.5 PSIA THROAT AREA = 2.32500E+00 SQ IN												
ISP = 2057.5 METERS/SEC = 209.8 LB-SEC/LB IVAC = 2245.2 METERS/SEC = 229.0 LB-SEC/LB												
CSTAR = 1558.8 FT/SEC THRUST COEFF = 4.3304 AREA RATIO = 6.333												
HEAT LOSS(QDOT/MDOT) = 1.0935E-02 CAL/(G-CM)												
CHEMICAL PROPERTIES												
SPECIES	MASS FRACTION	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE*CM**3/G**2/SEC)	NET RATE/POST- TIVE DIR RATE					
C3H8	5.56854E-07	2.10267E-07	3.30566E-08	1	3.8480E+00	-4.93770E+00	0.99992					
C2H5	1.56557E-05	1.39970E-05	3.50952E-06	2	4.8518E+10	3.80296E-03	0.99990					
CH3	1.45636E-04	2.51684E-04	-3.70288E-05	3	2.9365E+08	-7.65783E-02	0.04339					
CH4	6.30941E-04	1.02187E-03	2.24521E-05	4	2.3593E+01	-6.25179E+03	1.00000					
CSH7	2.02770E-11	1.22271E-11	5.38548E-10	5	8.8397E+11	-2.65015E+03	0.77877					
C2H4	2.07228E-04	1.91929E-04	-2.31085E-06	6	5.8032E+03	-3.87778E-02	0.99987					
H	9.82910E-05	2.53365E-05	-1.85952E-04	7	1.4368E+12	1.36498E+01	0.89058					
H2	3.87762E-03	4.99803E-02	8.23327E-05	8	3.0982E+12	2.57790E+02	0.79349					
O2	7.11964E-04	5.78104E-04	-9.71503E-04	9	1.5454E+08	3.26544E-02	0.98037					
H2O	3.96974E-07	3.10919E-07	1.56193E-08	10	6.3000E+12	-2.37944E+00	0.01441					
O	4.29184E-06	6.96981E-06	-1.55144E-06	11	7.9052E+09	6.13064E-03	0.77605					
NH	4.53450E-05	6.92747E-05	-2.30869E-05	12	1.40431E+13	1.31744E+03	0.99981					
H2O	1.02841E-01	1.48323E-01	1.39377E-05	13	2.3166E+12	1.01474E+03	0.99734					
CH3O	8.05791E-10	6.74628E-10	-5.73168E-10	14	4.2875E+12	5.17334E+00	0.99869					

TABLE D.2.—Continued.

(k) Continued.

CH20	3.36934E-05	2.91559E-05	2.76605E-06	15	2.0063E+13	2.40326E+02	0.99752
C2H6	1.35432E-04	1.17025E-04	3.83272E-07	16	2.4486E+11	-1.79301E+03	0.26100
CH2	7.14120E-06	1.32280E-05	-3.22903E-06	17	2.4890E+11	2.98311E+00	0.99994
C2H3	2.44702E-04	2.35083E-04	2.96100E-05	18	4.8000E+13	2.52151E+03	1.00000
C2H2	2.54527E-03	2.53987E-03	-3.01363E-05	19	2.0000E+13	9.86315E+01	1.00000
HC0	2.99220E-06	2.67917E-06	4.73737E-07	20	2.1373E+12	1.09689E+03	0.71248
C2H20	2.86666E-05	1.77184E-05	-2.00549E-07	21	1.1520E+03	-3.14093E-04	0.48954
C2H	1.62951E-07	1.69152E-07	-7.94274E-08	22	2.8748E+12	4.14227E+01	0.73161
C0	1.08064E-01	1.00241E-01	8.02278E-07	23	1.3405E+12	2.63897E+01	0.99957
C2H0	2.94028E-06	1.86198E-06	-4.13144E-07	24	2.0605E+12	4.08301E+00	1.00000
CH	4.95284E-07	9.88464E-07	-3.69731E-07	25	3.1112E+12	6.16304E+03	0.99970
C02	7.92424E-02	4.67832E-02	1.35748E-05	26	4.8421E+09	-9.80229E+00	0.85323
H202	1.47428E-08	1.12615E-08	-3.47037E-09	27	4.4171E+12	8.89198E+02	1.00000
H2	6.89184E-01	6.39222E-01	5.36243E-09	28	6.0000E+12	5.29367E+03	1.00000
HCN	2.97705E-05	2.86215E-05	1.36261E-09	29	3.3000E+13	8.00928E+01	1.00000
H	9.46478E-08	1.75572E-07	-6.57106E-09	30	5.0000E+12	1.20616E+02	1.00000
CN	2.73080E-09	2.72711E-09	-9.76126E-10	31	3.0000E+13	1.38189E+02	1.00000
HNCO	2.93575E-06	1.77288E-06	-6.56809E-08	32	3.0000E+13	1.76709E+00	1.00000
HC0	6.21521E-09	3.84336E-09	-1.28310E-09	33	1.8028E-03	-5.76105E+00	1.00000
NH2	3.11674E-05	5.05420E-05	6.69983E-08	34	2.5942E+12	6.80256E+01	1.00000
NO	1.25533E-04	1.08717E-04	9.90332E-09	35	4.7051E+12	1.23376E+02	0.99998
NH	2.85249E-07	4.93633E-07	6.13020E-10	36	3.4066E+11	-1.74895E-01	0.00197
N02	1.23908E-09	6.99794E-10	-1.50145E-12	37	2.9441E+11	7.66952E+01	0.99955
N20	3.77522E-08	2.22867E-08	-7.81921E-11	38	2.6759E+13	3.87603E+00	1.00000
HN02	3.55661E-08	1.96560E-08	-1.79580E-10	39	2.0000E+13	3.4713E-01	0.99994
HN03	1.17750E-13	4.85525E-14	7.88724E-15	40	5.1505E+11	8.21231E-01	1.00000
HN0	5.78710E-07	4.84825E-07	-1.35304E-08	41	1.2020E+12	2.31067E-02	1.00000
AR	1.17370E-02	7.63385E-03	0.00000E+00	42	1.0000E+13	1.91068E+00	1.00000
				43	5.0000E+13	3.49275E+02	0.99962
				44	3.0000E+13	1.09453E+00	1.00000
				45	4.3450E+12	1.58526E-01	1.00000
				46	1.0000E+13	5.13558E-02	1.00000
				47	2.8000E+13	5.09075E+01	0.99997
				48	2.1481E+12	3.54671E+00	0.90811
				49	2.7077E+12	1.80052E+02	0.99997
				50	2.6732E+12	1.60266E+02	0.90156
				51	1.7822E+12	3.10136E-01	0.95131
				52	2.0000E+13	3.65857E+00	1.00000
				53	2.7597E+05	-2.12019E+02	0.99997
				54	5.0000E+13	8.73185E-02	1.00000
				55	5.0374E+11	2.91014E-04	0.99999
				56	2.0000E+13	5.06385E-02	1.00000
				57	1.0908E+02	-1.12592E+00	1.00000
				58	1.8194E+13	5.44169E+01	0.99972
				59	4.7396E+12	5.18464E+02	0.99970
				60	8.1049E+12	2.43931E+00	0.99985
				61	2.8505E+10	3.09415E-01	0.99863
				62	1.0424E+13	1.04123E+01	1.00000
				63	2.0000E+13	2.31830E+00	1.00000
				64	5.1308E-01	-2.13862E+02	1.00000
				65	6.9894E+08	-2.72597E-01	0.29223
				66	5.2802E+08	4.13225E-04	0.50118
				67	6.9894E+08	-5.75676E-03	0.24180
				68	3.7000E+12	2.53449E+02	1.00000
				69	1.0000E+13	8.46456E+00	1.00000
				70	9.5526E+11	1.08208E+01	1.00000
				71	6.1442E+08	7.20734E-05	0.85893
				72	1.4859E+12	1.47994E+00	0.73376
				73	5.7926E+12	2.05554E+02	0.71479
				74	5.0000E+12	1.29597E+00	1.00000
				75	4.0000E+13	1.03678E+01	1.00000
				76	3.0000E+13	6.88273E+01	0.99999
				77	3.0000E+13	8.29810E-01	1.00000
				78	3.0000E+13	8.24770E+00	1.00000
				79	2.0000E+13	2.01101E+02	1.00000
				80	4.4074E+11	1.42434E+03	0.81431
				81	4.3461E+14	1.41695E+00	1.00000
				82	5.8334E+03	4.98748E-04	0.99604
				83	2.7487E+11	2.24808E+03	0.79510
				84	4.0670E+09	1.87760E-01	1.00000
				85	3.2240E+10	2.32112E+01	0.47015
				86	2.0324E+11	4.32438E+02	0.98066
				87	1.3629E+12	3.55427E+02	0.50540
				88	3.0014E+13	3.50218E+01	0.99997
				89	3.2958E+13	1.05795E-01	0.99999
				90	8.0000E+12	2.55234E-01	0.99997
				91	8.5789E+13	1.00107E+02	1.00000
				92	2.3611E+09	-8.04912E-01	0.93675
				93	3.3612E+12	3.65489E-03	0.94096
				94	1.8000E+12	2.57635E-04	0.99954
				95	7.8000E+11	3.29667E-02	1.00000
				96	8.3354E+08	-3.23303E-01	0.92791
				97	3.7327E+12	1.27344E+03	0.06652
				98	2.2149E+15	6.78746E+01	0.99996
				99	1.2115E-04	-9.99179E+01	1.00000
				100	5.8802E+15	4.84565E-01	1.00000
				101	9.2503E-04	-2.09776E+02	1.00000
				102	6.4783E-07	-1.71688E-05	1.00000
				103	3.6387E+07	3.40474E-02	0.99974
				104	6.5893E+12	1.23214E-01	0.09262
				105	1.5235E+10	2.04800E-03	0.45491
				106	1.2452E+11	2.70201E-01	0.73881
				107	1.2000E+13	3.37864E-04	1.00000
				108	2.0508E+13	4.51371E-03	0.78449
				109	2.3495E+12	-7.35703E-02	0.09914
				110	2.8939E+12	9.99988E+00	0.51934
				111	2.1093E+13	4.90565E-02	0.99587
				112	3.7000E+12	-2.93813E-02	0.04032
				113	2.0000E+13	7.93595E-04	1.00000
				114	1.0000E+13	9.99550E-04	1.00000
				115	2.0000E+13	2.88466E-01	0.99993
				116	2.5407E+11	4.04434E-02	1.00000
				117	2.0000E+12	3.18365E-01	1.00000
				118	7.5491E+12	3.79962E-01	0.99359
				119	2.5497E+12	1.27528E-01	0.99894
				120	7.8005E+12	5.55963E-05	0.98650
				121	9.1138E+15	3.22260E-02	1.00000
				122	1.8804E+14	4.93738E-01	0.99974
				123	1.9752E+05	-5.53383E-01	0.99985
				124	1.4913E+05	-5.96259E-02	1.00000

TABLE D.2.—Continued.
(k) Concluded.

	125	2.8432E+00	-8.22740E-01	1.00000		
	126	4.0000E+12	7.27987E-07	1.00000		
	127	2.3457E+04	-6.60741E-05	0.98842		
	128	8.4782E+08	1.95076E-07	1.00000		
	129	1.0471E+09	2.40855E-07	0.99966		
	130	1.4031E+11	1.17363E-02	1.00000		
	131	1.3525E+08	-3.34266E-01	0.99998		
	132	1.4619E+16	1.17722E-06	0.34903		
	133	1.1373E+16	3.07462E-01	0.76920		
	134	5.0000E+12	9.09786E+00	1.00000		
	135	6.9342E+15	8.86939E+00	0.99509		
	136	3.6000E+13	1.79102E+00	1.00000		
DERIVATIVES (CGS UNITS): $\dot{T}$	-8.25079E+01	RHO	-1.95264E-05	V	5.76675E+03	
MIXTURE MOLECULAR WEIGHT	25.98253	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	-2.08273E+09	MASS FRACTION SUM	1.00000017	

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 8.799896E-01 S UP TO THIS TIME - 1.016998E+01 S

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS -	158
TOTAL NO. OF DERIVATIVE EVALUATIONS -	203
TOTAL NO. OF JACOBIAN EVALUATIONS -	30
TOTAL CPU TIME -	10.169983 S

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 12.259995 S

(LSENS) READ DATA FOR NEXT CASE

TABLE D.2.—Continued.
(I) Case 12

DISTANCE-AREA VERSION				LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM				NASA LEWIS RESEARCH CENTER			
LSENS HIGH TEMPERATURE AIR IONIZATION				CASE 12							
REACTION NUMBER		REACTION				REACTION RATE VARIABLES		ACTIVATION ENERGY			
1	1*N	+	1*O2	=	1*N*O	+	1*O	6.40000E+09	1.0000		
2	1*O	+	1*N2	=	1*N*O	+	1*N	1.80000E+14	0.0000		
3	1*N	+	1*O	=	1*N*O	+	M	6.40000E+16	-0.5000		
4			2*O	=	1*O2	+	M	5.70000E+13	0.0000		
5	M	+	1*N2	=	2*N			3.72000E+21	-1.6000		
6	1*N*O	+	1*O	=	1*N*O2	+	M	5.62000E+15	0.0000		
7	M	+	1*N2O	=	1*N2	+	1*O	6.92000E+23	-2.5000		
8	1*O	+	1*N2O	=	1*N2	+	1*O2	1.00000E+14	0.0000		
9	1*N*O+	+	1*N	=	1*N	+	1*O	1.45000E+21	-1.5000		
10	1*O+	+	1*N	=	1*O	+	M	2.00000E+26	-2.5000		
11	1*O2	+	1*N	=	1*O2-	+	M	1.52000E+21	-1.0000		
12	1*O2	+	1*O-	=	1*O2-	+	1*O	6.00000E+12	0.0000		
									1190.00		
									0.00		
ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING											
M(H2O	, 3) =	2.25000	M(N2	, 6) =	1.55000	M(O2	, 10) =	4.50000	M(N	, 10) =	0.03000
M(HO	, 10) =	50.00000	M(O	, 10) =	0.03000	M(N2	, 11) =	0.00002			
** INITIAL CONDITIONS **											
TIME	0.00000E+00	SEC	AREA	1.00000E+03	SQ CM	AXIAL POSITION	0.00000E+00	CM			
FLOW PROPERTIES						INTEGRATION INDICATORS					
PRESSURE (ATM)		1.68030	STEPS FROM LAST PRINT						0		
VELOCITY (CM/SEC)		47002.00	AVERAGE STEP SIZE						0.00000E+00		
DENSITY (G/CM**3)		1.22560E-04	METHOD ORDER						0		
TEMPERATURE (DEG K)		4820.00	TOTAL NUMBER OF STEPS						0		
MASS FLOW RATE (G/SEC)		5.76058E+03	FUNCT EVALUATIONS						0		
ENTROPY (CAL/G/DEG K)		2.3905	JACOBIAN EVALUATIONS						0		
MACH NUMBER		0.3535									
GAMMA		1.2726									
ENTHALPY (CAL/G)		1.35458E+03									
SP. HEAT (CP) (CAL/G/DEG K)		3.21566E-01									
CHEMICAL PROPERTIES											
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE				
N	0.00000E+00	0.00000E+00	8.53190E-06	1	1.6063E+13	0.00000E+00	0.00000				
O2	8.90048E-07	2.09500E-01	-2.31733E-02	2	6.2795E+10	0.00000E+00	0.00000				
NO	0.00000E+00	0.00000E+00	0.00000E+00	3	9.2184E+14	0.00000E+00	0.00000				
O	0.00000E+00	0.00000E+00	4.33027E-02	4	6.8713E+13	-1.34005E+06	1.00000				
N2	3.35839E-06	7.90500E-01	-5.04911E-03	5	2.8989E+05	2.83988E+02	1.00000				
NO2	0.00000E+00	0.00000E+00	0.00000E+00	6	6.3436E+15	0.00000E+00	0.00000				
N2O	0.00000E+00	0.00000E+00	3.0484E-03	7	4.8444E+11	0.00000E+00	0.00000				
NO+	0.00000E+00	0.00000E+00	0.00000E+00	8	5.3643E+12	-2.02705E+05	0.00000				
E	0.00000E+00	0.00000E+00	4.38522E-07	9	4.3331E+15	0.00000E+00	0.00000				
O+	0.00000E+00	0.00000E+00	0.00000E+00	10	1.2400E+17	0.00000E+00	0.00000				
O2-	4.24844E-15	1.00000E-09	-4.38522E-07	11	2.7851E+17	-2.91938E+01	1.00000				
O-	0.00000E+00	0.00000E+00	0.00000E+00	12	6.0000E+12	0.00000E+00	0.00000				
DERIVATIVES (CGS UNITS): T			-1.49460E+03	RHO	2.89845E-05	V	-1.11156E+04				
MIXTURE MOLECULAR WEIGHT		28.84834	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)		1.79700E+11	MASS FRACTION SUM		1.00000000			
SPECIES MOLE NUMBERS (MOLE SPECIES I/G MIXTURE) AND DERIVATIVES (CGS UNITS: MOLE SPECIES I/G MIXTURE/S OR CM)											
SPECIES	SIGMA(I)	DSIGMA(I)/DIVAR	SPECIES	SIGMA(I)	DSIGMA(I)/DIVAR	SPECIES	SIGMA(I)	DSIGMA(I)/DIVAR			
N	0.00000E+00	0.14811E-05	O2	0.72621E-02	-0.40271E-02	NO	0.00000E+00	0.00000E+00			
O	0.00000E+00	0.75171E-02	N2	0.27402E-01	-0.52911E-03	NO2	0.00000E+00	0.00000E+00			
N2O	0.00000E+00	0.52856E-03	NO+	0.00000E+00	0.00010E+00	E	0.00000E+00	0.76123E-07			
O+	0.00000E+00	0.00000E+00	O2-	0.34664E-10	-0.76123E-07	O-	0.00000E+00	0.00000E+00			

TABLE D.2.—Continued.

(1) Continued.

SPECIES	OMEGA(I,J) RATE OF PRODUCTION OF SPECIES I BY REACTION J (MOLE SPECIES I/CC/S)							
	1	2	3	4	5	6	7	8
	9	10	11	12				
N	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.85319E-05	0.00000E+00	0.00000E+00	0.00000E+00
O2	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.43852E-06	-0.20129E-01 0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	-0.30448E-02
NO	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
O	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.40258E-01 0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.30448E-02
H2	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	-0.42659E-05	0.00000E+00	0.00000E+00	-0.30448E-02
NO2	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
H2O	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.30448E-02
NO+	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
E	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.43852E-06	0.00000E+00 0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
O+	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
O2-	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 -0.43852E-06	0.00000E+00 0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
O-	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

CPU TIME FOR INITIALIZATION OF LSENS = 0.949997 S

TIME 1.59489E-05 SLC AREA 1.00000E+03 SQ CM AXIAL POSITION 7.00000E-01 CM

FLOW PROPERTIES

PRESSURE 1.70904
(ATM)
VELOCITY 41946.49
(CM/SEC)
DENSITY 1.37332E-04
(G/CM**3)
TEMPERATURE 4238.68
(DEG K)
MASS FLOW RATE 5.76058E+03
(G/SEC)
ENTROPY 2.4163
(CAL/G/DEG K)
MACH NUMBER 0.3292
GAMMA 1.2873
ENTHALPY 1.35995E+03
(CAL/G)
SP. HEAT (CP) 5.18551E-01
(CAL/G/DEG K)

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 4
AVERAGE STEP SIZE 0.50398E-01
METHOD ORDER 4
TOTAL NUMBER OF STEPS 57
FUNCT EVALUATIONS 73
JACOBIAN EVALUATIONS 14

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSTIVE DIR RATE
N	1.44559E-09	2.94154E-04	-2.40893E-05	1	1.29171E+13	2.93986E+05	0.44160
O2	6.72505E-07	1.36862E-01	-9.27740E-03	2	2.1075E+10	2.85929E+05	0.23345
NO	3.44095E-07	7.00273E-02	1.08092E-02	3	9.8302E+14	-6.75873E+03	0.98355
O	3.05299E-07	6.21318E-02	7.75744E-03	4	7.0497E+13	-1.84687E+05	0.99082
H2	3.59017E-06	7.30639E-01	-5.37990E-03	5	1.4649E+10	1.35292E+01	0.98739
NO2	1.13223E-11	2.30421E-06	5.15564E-07	6	6.4498E+15	2.73364E+01	0.00011
H2O	2.06908E-10	4.21081E-05	-1.29661E-05	7	2.6338E+11	1.39241E+04	0.98071
NO+	1.54269E-12	3.13954E-07	1.06516E-07	8	3.5914E+12	-1.32566E+04	0.52390
E	1.53645E-12	3.12686E-07	1.05370E-07	9	5.2544E+15	-5.64771E+00	0.89532
O+	2.74119E-18	5.57863E-13	8.04637E-14	10	1.7098E+17	-4.26638E-06	0.99979
O2-	5.47934E-15	7.08084E-10	2.43515E-10	11	3.1135E+17	6.07560E-02	0.00269
O-	7.51715E-15	1.52983E-09	9.02342E-10	12	6.0000E+12	-4.78443E-02	0.02889

DERIVATIVES (CGS UNITS): T -3.73835E+02 RHO 1.10772E-05 V -5.38345E+03

MIXTURE MOLECULAR WEIGHT 27.94853 TOTAL ENERGY EXCHANGE RATE 3.68408E+10 MASS FRACTION SUM 1.00000002
(CAL-CM**3/G**2/SEC)

SPECIES MOLE NUMBERS (MOLE SPECIES I/G MIXTURE) AND DERIVATIVES (CGS UNITS) MOLE SPECIES I/G MIXTURE/S OR CM

SPECIES	SIGMA(I)	DSIGMA(I)/DIVAR	SPECIES	SIGMA(I)	DSIGMA(I)/DIVAR	SPECIES	SIGMA(I)	DSIGMA(I)/DIVAR
N	0.10525E-04	-0.41818E-05	O2	0.48969E-02	-0.16105E-02	NO	0.25056E-02	0.18764E-02
O	0.22231E-02	0.13666E-02	H2	0.26142E-01	-0.93392E-03	NO2	0.82445E-07	0.89499E-07
H2O	0.15066E-05	-0.22508E-05	NO+	0.11233E-07	0.18490E-07	E	0.11188E-07	0.18292E-07
O+	0.19960E-13	0.13968E-13	O2-	0.25335E-10	0.42273E-10	O-	0.54737E-10	0.15664E-09

TABLE D.2.—Continued.
(I) Continued.

SPECIES	OMEGA(I,J) RATE OF PRODUCTION OF SPECIES I BY REACTION J (MOLE SPECIES I/CC/S)							
	1	2	3	4	5	6	7	8
	9	10	11	12				
H	-0.55446E-02 -0.10652E-06	0.53926E-02 0.00000E+00	0.12747E-03 0.00000E+00	0.00000E+00 0.00000E+00	0.51032E-06	0.00000E+00	0.00000E+00	0.00000E+00
O2	-0.55446E-02 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 -0.11459E-08	-0.34832E-02 0.90234E-09	0.00000E+00	0.00000E+00	0.00000E+00	-0.24964E-03
HO	0.55446E-02 0.00000E+00	0.53926E-02 0.00000E+00	-0.12747E-03 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00	-0.51556E-06	0.00000E+00	0.00000E+00
O	0.55446E-02 -0.10652E-06	-0.53926E-02 -0.80464E-13	0.12747E-03 0.00000E+00	0.69664E-02 -0.90234E-09	0.00000E+00	-0.51556E-06	0.26261E-03	0.24964E-03
N2	0.00000E+00 0.00000E+00	-0.53926E-02 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	-0.25516E-06	0.00000E+00	0.26261E-03	-0.24964E-03
N02	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00	0.51556E-06	0.00000E+00	0.00000E+00
N2O	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00	0.00000E+00	-0.26261E-03	0.24964E-03
NO+	0.00000E+00 0.10652E-06	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
E	0.00000E+00 0.10652E-06	0.00000E+00 0.80464E-13	0.00000E+00 -0.11459E-08	0.00000E+00 0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
O+	0.00000E+00 0.00000E+00	0.00000E+00 0.80464E-13	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
O2-	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.11459E-08	0.00000E+00 -0.90234E-09	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
O-	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.00000E+00	0.00000E+00 0.90234E-09	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 3.999329E-02 S UP TO THIS TIME - 3.999939E-01 S

TIME 1.59489E-05 SEC AXIAL POSITION 7.00000E-01 CM

REACTION IMPORTANCE FOR SPECIES FORMATION AND RATES

SPECIES (I)	REACTION NUMBER (J)									
	OMEGA(I,J) RATE OF PRODUCTION OF SPECIES I BY REACTION J (MOLE/CM**3/S)									
N	1	2	3	5	9					
	-5.545E-03	5.393E-03	1.275E-04	5.103E-07	-1.065E-07					
O2	1	4	8	11	12					
	-5.545E-03	-3.483E-03	-2.496E-04	-1.146E-09	9.023E-10					
NO	1	2	3	6						
	5.545E-03	5.393E-03	-1.275E-04	-5.156E-07						
O	4	1	2	7	8	3	6	9	12	10
	6.966E-03	5.545E-03	-5.393E-03	2.626E-04	2.496E-04	1.275E-04	-5.156E-07	-1.065E-07	-9.023E-10	-8.046E-14
N2	2	7	8	5						
	-5.393E-03	2.626E-04	-2.496E-04	-2.552E-07						
NO2	6									
	5.156E-07									

TABLE D.2.—Continued.
(1) Concluded.

	7	8	
N20	-2.626E-04	2.496E-04	
	9		
H0+	1.065E-07		
	9	11	10
E	1.065E-07	-1.146E-09	8.046E-14
	10		
0+	8.046E-14		
	11	12	
02-	1.146E-09	-9.023E-10	
	12		
0-	9.023E-10		

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM.

TOTAL NO. OF STEPS -	57
TOTAL NO. OF DERIVATIVE EVALUATIONS -	73
TOTAL NO. OF JACOBIAN EVALUATIONS -	14
TOTAL CPU TIME -	0.399994 S

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 1.910004 S

(LSENS) READ DATA FOR NEXT CASE

(m) Case 13

[illegible]

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** EQUILIBRIUM CALCULATION **

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THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED TEMPERATURE AND DENSITY

	INITIAL STATE	FINAL STATE	FINAL/INITIAL RATIO
PRESSURE (ATM)	100.0000	98.0001	0.9800
VELOCITY (CM/SEC)	0.00	0.00	1.0000
DENSITY (G/CM**3)	2.77341E-03	2.77341E-03	1.0000
TEMPERATURE (DEG K)	1000.00	1000.00	1.0000
ENTHALPY (CAL/G)	2057.01343	1820.27039	0.88491
INTERNAL ENERGY (CAL/G)	1183.82056	966.34108	0.81477
SP. HEAT (CP) (CAL/G/DEG K)	3.17527	3.16527	0.99685
ENTROPY (CAL/G/DEG K)	13.5443	13.4256	0.9912
MACH NUMBER	0.0000	0.0000	1.0000
GAMMA	1.3793	1.3705	0.9936
SONIC VELOCITY (CM/SEC)	224481.86	221517.32	0.9868

SPECIES	MOLE FRACTION
CH3	2.32219E-11
OH	2.32219E-11
CH3O	2.32219E-11
H	2.32219E-11
CH2O	2.32219E-11
H2	9.79592E-01
HC0	2.32219E-11
CH4	1.02038E-02
CO	2.86966E-07
HNO2	2.32219E-11
H2O	1.02038E-02
CO2	2.32219E-11
H2O2	2.32219E-11

MIXTURE MOLECULAR WEIGHT	2.2219
D(LOG VOLUME)/D(LOG T) AT CONSTANT P	1.0000
D(LOG VOLUME)/D(LOG P) AT CONSTANT T	-1.0000

COMPUTATIONAL WORK REQUIRED FOR EQUILIBRIUM CALCULATION:
NO. OF ITERATIONS = 11 CPU TIME = 2.000427E-02 S

TABLE D.2.—Continued.
(m) Continued.

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM										NASA LEWIS RESEARCH CENTER	
LSENS HIGH PRESSURE HYDROGEN - CARBON MONOXIDE REACTION										CASE 13	
REACTION NUMBER	REACTION					REACTION RATE VARIABLES		ACTIVATION ENERGY			
						A	H				
1	1*CH3	+	1*OH	=	1*CH3O	+	1*H	6.30000E+12	0.0000	0.00	
2	M	+	1*CH3O	=	1*CH2O	+	1*H	5.00000E+13	0.0000	21000.00	
3	1*CH3O	+	1*H	=	1*CH2O	+	1*H2	2.00000E+13	0.0000	0.00	
4	1*CH3	+	1*HCO	=	1*CH4	+	1*CO	3.00000E+11	0.5000	0.00	
5	1*CH3	+	1*H2O	=	1*CH3O	+	1*OH	2.00000E+13	0.0000	0.00	
6	M	+	1*CH4	=	1*CH3	+	1*H	2.00000E+17	0.0000	88000.00	
7	1*H	+	1*CH4	=	1*CH3	+	1*H2	1.26000E+14	0.0000	11900.00	
8	1*OH	+	1*CH4	=	1*CH3	+	1*H2O	2.50000E+13	0.0000	5010.00	
9	1*CH2O	+	1*H	=	1*HCO	+	1*H2	2.50000E+13	0.0000	3990.00	
10	1*CH2O	+	1*OH	=	1*HCO	+	1*H2O	3.00000E+13	0.0000	1200.00	
11	M	+	1*CH2O	=	1*H	+	1*HCO	5.00000E+16	0.0000	81000.00	
12	1*HCO	+	1*H	=	1*CO	+	1*H2	2.00000E+13	0.0000	0.00	
13	1*HCO	+	1*OH	=	1*CO	+	1*H2O	3.00000E+13	0.0000	0.00	
14	M	+	1*HCO	=	1*H	+	1*CO	2.90000E+14	0.0000	15570.00	
15	1*CO	+	1*OH	=	1*CO2	+	1*H	4.17000E+11	0.0000	1000.00	
16	1*CO	+	1*H2O	=	1*CO2	+	1*OH	5.75000E+13	0.0000	22930.00	
17	1*H	+	1*H2O	=	2*OH			1.36000E+14	0.0000	1070.00	
18	1*H2	+	1*H2O	=	1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00	
19	1*OH	+	1*H2O2	=	1*H2O	+	1*H2O	6.10000E+12	0.0000	1430.00	
20	M	+	1*H2O2	=	2*OH			1.46000E+17	0.0000	45510.00	
21	1*H2	+	1*OH	=	1*H2O	+	1*H	4.74000E+13	0.0000	6098.00	
22	M	+	1*H2O	=	1*H	+	1*OH	1.30000E+15	0.0000	105140.00	
23	M	+	1*H2	=	2*H			2.20000E+14	0.0000	96000.00	

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	, 20) =	2.30000	M(H2O2	, 20) =	6.60000	M(H2O	, 20) =	6.00000	M(H2	, 22) =	4.00000
M(CO2	, 22) =	4.00000	M(H2O	, 22) =	20.00000	M(H2	, 23) =	4.10000	M(H2O	, 23) =	15.00000

*** INITIAL CONDITIONS ***

TIME	0.00000E+00	SEC	AREA	0.00000E+00	SQ CM	AXIAL POSITION	0.00000E+00	CM
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FLOW PROPERTIES				INTEGRATION INDICATORS			
PRESSURE (ATM)	100.00000	STEPS FROM LAST PRINT	0				
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE	0.00000E+00				
DENSITY (G/CM**3)	2.77341E-03	METHOD ORDER	0				
TEMPERATURE (DEG K)	1000.00						
MASS FLOW RATE (G/SEC)	0.00000E+00	TOTAL NUMBER OF STEPS	0				
ENTROPY (CAL/G/DEG K)	13.5443	FUNCT EVALUATIONS	0				
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS	0				
GAMMA	1.3793						
ENTHALPY (CAL/G)	2.05701E+03						
SP. HEAT (CP) (CAL/G/DEG K)	3.17527E+00						

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIONAL DIR RATE
CH3	0.00000E+00	0.00000E+00	0.00000E+00	1	6.3000E+12	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	0.00000E+00	2	1.2865E+09	0.00000E+00	0.00000
CH3O	0.00000E+00	0.00000E+00	0.00000E+00	3	2.0000E+13	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	2.79263E-12	4	9.4868E+12	0.00000E+00	0.00000
CH2O	0.00000E+00	0.00000E+00	0.00000E+00	5	2.0000E+13	0.00000E+00	0.00000
H2	1.20649E-03	9.90000E-01	-1.41686E-12	6	1.1712E-02	0.00000E+00	0.00000
HCO	0.00000E+00	0.00000E+00	4.10895E-14	7	3.1596E+11	0.00000E+00	0.00000
CH4	0.00000E+00	0.00000E+00	0.00000E+00	8	2.0091E+12	0.00000E+00	0.00000
CO	1.21868E-05	1.00000E-02	-4.10895E-14	9	3.3568E+12	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	10	1.6401E+13	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	11	9.9183E-02	0.00000E+00	0.00000
CO2	0.00000E+00	0.00000E+00	0.00000E+00	12	2.0000E+13	-5.36200E-09	1.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	13	3.0000E+13	0.00000E+00	0.00000
				14	1.1470E+11	0.00000E+00	0.00000
				15	2.5211E+11	0.00000E+00	0.00000
				16	5.6017E+08	0.00000E+00	0.00000
				17	7.8209E+13	0.00000E+00	0.00000
				18	2.7191E+08	0.00000E+00	0.00000
				19	2.9703E+12	0.00000E+00	0.00000
				20	1.6299E+07	0.00000E+00	0.00000
				21	2.2032E+12	0.00000E+00	0.00000
				22	1.3665E+08	0.00000E+00	0.00000
				23	2.2996E-07	1.78862E-07	1.00000

DERIVATIVES (CGS UNITS), T

	0.00000E+00	RHO	0.00000E+00
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MIXTURE MOLECULAR WEIGHT

2.27575	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	1.91134E-02	MASS FRACTION SUM	1.00000000
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CPU TIME FOR INITIALIZATION OF LSENS = 1.049988 S

TABLE D.2.—Continued.
(m) Concluded.

TIME	1.00000E+09	SEC	AREA	0.00000E+00	SQ CM	AXIAL POSITION	0.00000E+00	CM
FLOW PROPERTIES			INTEGRATION INDICATORS					
PRESSURE (ATM)	98.00324		STEPS FROM LAST PRINT	32				
VELOCITY (CM/SEC)	0.00		AVERAGE STEP SIZE	0.28531E+08				
DENSITY (G/CM**3)	2.77341E-03		METHOD ORDER	4				
TEMPERATURE (DEG K)	1000.00							
MASS FLOW RATE (G/SEC)	0.00000E+00		TOTAL NUMBER OF STEPS	122				
ENTROPY (CAL/G/DEG K)	13.4259		FUNCT EVALUATIONS	161				
MACH NUMBER	0.0000		JACOBIAN EVALUATIONS	30				
GAMMA	1.3706							
ENTHALPY (CAL/G)	1.82065E+03							
SP. HEAT (CP) (CAL/G/DEG K)	5.16510E+00							
CHEMICAL PROPERTIES								
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RAIL/POSTIVE DIR RATE	
CH3	5.61735E-14	4.70329E-11	-2.46945E-13	1	6.3000E+12	-1.60532E-11	0.98183	
OH	6.45768E-18	5.40687E-15	-4.00448E-15	2	1.2865E+09	-1.61333E-11	0.03179	
CH3O	2.45959E-21	2.05936E-18	6.16723E-19	3	2.0000E+13	-5.65353E-17	0.00016	
H	2.69224E-13	2.25416E-10	-1.18634E-14	4	9.4868E+12	-1.33068E-16	0.00016	
CH2O	2.54826E-12	2.13360E-09	-3.30179E-16	5	2.0000E+13	-2.77355E-24	0.98182	
H2	1.16999E-03	9.79609E-01	-2.51061E-13	6	1.1712E-02	5.80922E-12	0.00000	
HCO	1.17880E-17	9.86985E-15	2.62903E-13	7	3.1596E+11	-3.21271E-08	0.00000	
CH4	1.21671E-05	1.01872E-02	-2.47068E-13	8	2.0091E+12	2.17912E-13	0.00000	
CO	1.94159E-08	1.62565E-05	-2.62672E-13	9	3.3568E+12	2.67861E-11	0.00009	
HO2	3.51516E-31	2.94317E-28	-6.64869E-32	10	1.6401E+13	3.14786E-15	0.00009	
H2O	1.21668E-05	1.01870E-02	4.15303E-15	11	9.9183E-02	3.55072E-15	0.00009	
CO2	2.91174E-10	2.43794E-07	-2.50644E-17	12	2.0000E+13	-1.36648E-15	0.00016	
H2O2	3.25150E-26	2.72241E-23	1.43246E-27	13	3.0000E+13	-4.83715E-20	0.00016	
				14	1.1470E+11	-3.41529E-08	0.00016	
				15	2.5211E+11	-3.25859E-12	0.00079	
				16	5.6017E+08	-2.99657E-28	0.00060	
				17	7.8209E+13	1.82740E-28	0.00019	
				18	2.7191E+08	2.78229E-24	0.00019	
				19	2.9703E+12	-1.54997E-29	0.00019	
				20	1.6299E+07	-1.85450E-22	0.00000	
				21	2.2032E+12	5.39709E-10	0.00000	
				22	1.3665E-08	2.68750E-17	0.00000	
				23	2.2996E-07	8.75260E-14	0.00000	
DERIVATIVES (CGS UNITS): T								
	0.00000E+00		KHO	0.00000E+00				
MIXTURE MOLECULAR WEIGHT	2.32211		TOTAL ENERGY EXCHANGE RATE	-5.50202E-04		MASS FRACTION SUM	1.00000000	
(CAL-CM**3/G**2/SEC)								
COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 1.499939E-01 S UP TO THIS TIME - 6.199951E-01 S								
(LENS) END OF THIS CASE								
SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:								
	TOTAL NO. OF STEPS -	122						
	TOTAL NO. OF DERIVATIVE EVALUATIONS -	161						
	TOTAL NO. OF JACOBIAN EVALUATIONS -	30						
	TOTAL CPU TIME -	0.619995 S						
TOTAL CPU TIME (INCLUDING I/O) REQUIRED - 2.089996 S								
(LENS) READ DATA FOR NEXT CASE								

(n) Case 14

XX DATA LINES XX

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED INTERNAL ENERGY AND DENSITY

SPECIES	MOLE FRACTION
O	4.05365E-02
H2O	5.23165E-01
OH	1.33129E-01
H	8.74128E-02
O2	5.02276E-02
H2	1.65334E-01
H2O2	1.87876E-04
H2O2	1.08549E-05

NO. OF ITERATIONS =

TABLE D.2.—Continued.
(n) Continued.

MM INITIAL CONDITIONS MM									
TIME	0.00000E+00	SEC	AREA	0.00000E+00	SQ CM	AXIAL POSITION	0.00000E+00	CM	
FLOW PROPERTIES					INTEGRATION INDICATORS				
PRESSURE (ATM)	2.00000				STEPS FROM LAST PRINT	0			
VELOCITY (CM/SEC)	0.00				AVERAGE STEP SIZE	0.00000E+00			
DENSITY (G/CM**3)	4.17838E-04				METHOD ORDER	0			
TEMPERATURE (DEG K)	700.00								
MASS FLOW RATE (G/SEC)	0.00000E+00				TOTAL NUMBER OF STEPS	0			
ENTROPY (CAL/G/DEG K)	3.5907				FUNCT EVALUATIONS	0			
MACH NUMBER	0.0000				JACOBIAN EVALUATIONS	0			
GAMMA	1.3728								
ENTHALPY (CAL/G)	2.38986E+02								
SP. HEAT (CP) (CAL/G/DEG K)	6.09751E-01								
CHEMICAL PROPERTIES									
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST COS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE		
O	0.00000E+00	0.00000E+00	1.15949E-07	1	1.2552E+08	0.00000E+00	0.00000		
H2O	0.00000E+00	0.00000E+00	0.00000E+00	2	1.4327E+09	0.00000E+00	0.00000		
OH	0.00000E+00	0.00000E+00	0.00000E+00	3	2.1395E+10	0.00000E+00	0.00000		
H	0.00000E+00	0.00000E+00	1.39348E-07	4	1.5789E+13	-2.31827E-06	1.00000		
O2	1.15949E-05	3.33000E-01	-5.79748E-08	5	2.4364E+13	0.00000E+00	0.00000		
H2	2.32246E-05	6.67000E-01	-6.96741E-08	6	8.0000E+12	0.00000E+00	0.00000		
HO2	0.00000E+00	0.00000E+00	0.04743E-13	7	6.2092E+13	0.00000E+00	0.00000		
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	8	1.2383E+06	0.00000E+00	0.00000		
				9	2.1820E+12	0.00000E+00	0.00000		
				10	1.8000E+12	0.00000E+00	0.00000		
				11	7.8000E+11	0.00000E+00	0.00000		
				12	8.9025E+02	0.00000E+00	0.00000		
				13	5.9142E+11	0.00000E+00	0.00000		
				14	2.9962E+15	0.00000E+00	0.00000		
				15	1.9398E-18	0.00000E+00	0.00000		
				16	1.0143E+16	0.00000E+00	0.00000		
				17	2.3436E-16	3.69149E-18	1.00000		
				18	3.6533E-22	8.44979E-25	1.00000		
				19	3.0000E-03	3.99074E-01	1.00000		
				20	5.0000E-03	3.32063E-01	1.00000		
DERIVATIVES (COS UNITS): T			-7.61641E+01	RHO	0.00000E+00				
MIXTURE MOLECULAR WEIGHT		12.00014	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)		8.13371E+04	MASS FRACTION SUM		1.00000000	
CPU TIME FOR INITIALIZATION OF LSENS =					0.949997 S				
TIME	1.01636E+00	SEC	AREA	0.00000E+00	SQ CM	AXIAL POSITION	0.00000E+00	CM	
FLOW PROPERTIES					INTEGRATION INDICATORS				
PRESSURE (ATM)	2.69601				STEPS FROM LAST PRINT	100			
VELOCITY (CM/SEC)	0.00				AVERAGE STEP SIZE	0.51403E-02			
DENSITY (G/CM**3)	4.17838E-04				METHOD ORDER	4			
TEMPERATURE (DEG K)	956.82								
MASS FLOW RATE (G/SEC)	0.00000E+00				TOTAL NUMBER OF STEPS	200			
ENTROPY (CAL/G/DEG K)	3.7233				FUNCT EVALUATIONS	295			
MACH NUMBER	0.0000				JACOBIAN EVALUATIONS	36			
GAMMA	1.3529								
ENTHALPY (CAL/G)	2.79326E+02								
SP. HEAT (CP) (CAL/G/DEG K)	6.26068E-01								
CHEMICAL PROPERTIES									
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST COS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE		
O	1.62898E-12	4.74388E-08	1.42767E-09	1	3.3420E+09	3.19301E-02	0.99639		
H2O	7.91009E-07	2.30355E-02	1.10181E-04	2	3.3922E+10	6.40247E+01	1.00000		
OH	2.51101E-12	7.31248E-08	1.70843E-09	3	5.0378E+11	6.33436E+01	1.00000		
H	2.96556E-11	8.63623E-07	2.47190E-08	4	2.3797E+13	1.86430E+01	0.99555		
O2	1.11117E-05	3.23593E-01	-4.94514E-05	5	2.9550E+13	1.27731E+00	1.00000		
H2	2.25482E-05	6.50819E-01	-1.03666E-04	6	8.0000E+12	5.33040E-01	1.00000		
HO2	4.63275E-09	1.34914E-04	1.77515E-06	7	6.331E+13	6.00665E+01	1.00000		
H2O2	8.29927E-08	2.41689E-03	-7.41585E-06	8	5.411E+08	-6.74639E+01	0.42469		
				9	8.754E+12	3.43084E+00	0.99961		
				10	8.000E+12	2.19563E+02	0.99226		
				11	8.000E+11	1.09958E+01	1.00000		
				12	7.976E+06	1.80149E+02	1.00000		
				13	9.183E+12	6.16155E+02	0.99952		
				14	4.704E+15	4.58919E+02	0.99997		
				15	2.546E-09	-6.89258E-03	1.00000		
				16	7.4205E+15	7.05052E-05	1.00000		
				17	2.5984E-08	-2.83597E-03	1.00000		
				18	2.0751E-12	-5.4156E-08	1.00000		
				19	3.0000E-03	3.84015E-01	1.00000		
				20	5.0000E-03	3.18227E-01	1.00000		
DERIVATIVES (COS UNITS): T			3.19339E+04	RHO	0.00000E+00				
MIXTURE MOLECULAR WEIGHT		12.16816	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)		-3.50.69E+07	MASS FRACTION SUM		1.00000001	
COMPUTER TIME (CPU) REQUIRED FOR THIS STEP - 6.699982E-01 S UP TO THIS TIME - 1.2400051E+00 S									

TABLE D.2.—Continued.
(n) Concluded.

TIME	1.01730E+00	SEC	AREA	0.00000E+00	SQ CM	AXIAL POSITION	0.00000E+00	CM
FLOW PROPERTIES					INTEGRATION INDICATORS			
PRESSURE (ATM)	2.88438		STEPS FROM LAST PRINT		32			
VELOCITY (CM/SEC)	0.00		AVERAGE STEP SIZE		0.29456E-04			
DENSITY (G/CM**3)	4.17838E-04		METHOD UNDER		4			
TEMPERATURE (DEG K)	1026.93		TOTAL NUMBER OF STEPS		232			
MASS FLOW RATE (G/SEC)	0.00000E+00		FUNCT EVALUATIONS		349			
ENTROPY (CAL/G/DEG K)	3.7533		JACOBIAN EVALUATIONS		41			
MACH NUMBER	0.0000							
GAMMA	1.3477							
ENTHALPY (CAL/G)	2.90243E+02							
SP. HEAT (CP) (CAL/G/DEG K)	6.30997E-01							
CHEMICAL PROPERTIES								
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSI- TIVE DIR RATE	
O	1.18540E-11	3.46311E-07	9.14943E-08	1	8.3967E+09	5.83952E-01	0.99108	
H2O	1.03350E-06	3.01934E-02	8.87724E-04	2	6.1129E+10	7.69581E+02	0.99998	
OH	1.65441E-11	4.83332E-07	1.45325E-07	3	4.9774E+11	7.47452E+02	0.99999	
H	1.99828E-10	5.83791E-06	1.47962E-06	4	2.5685E+13	3.05426E+02	0.99808	
O2	1.09995E-05	3.21347E-01	-4.19885E-04	5	3.0630E+13	2.16481E+01	1.00000	
H2	2.21176E-05	6.46157E-01	-8.49624E-04	6	8.0000E+12	7.89108E+00	1.00000	
HO2	1.04092E-08	3.04102E-04	2.96330E-05	7	7.9321E+13	9.45039E+02	1.00000	
H2O2	6.81766E-08	1.99175E-03	-5.37281E-05	8	3.7821E+08	-5.72629E+02	0.53449	
				9	3.0269E+12	1.95408E+01	0.99926	
				10	1.8000E+12	1.11250E+03	0.99588	
				11	7.8000E+11	6.08654E+01	1.00000	
				12	2.9718E+07	7.67210E+02	1.00000	
				13	2.3879E+12	4.99676E+03	0.99841	
				14	2.3833E+15	3.08257E+03	0.99993	
				15	5.4735E-08	-1.88330E-01	1.00000	
				16	6.9138E+15	3.21086E-03	1.00000	
				17	8.1639E-07	-9.76464E-02	1.00000	
				18	1.3395E-10	-2.58887E-06	1.00000	
				19	3.0000E-03	3.80052E-01	1.00000	
				20	5.0000E-03	3.15013E-01	1.00000	
DERIVATIVES (CGS UNITS): T			2.55051E+05	RHO	0.00000E+00			
MIXTURE MOLECULAR HEIGHT		12.20699	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)		-2.83276E+08	MASS FRACTION SUM	1.00000001	
COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 2.200012E-01 S UP TO THIS TIME - 1.460007E+00 S								
(LSEHS) END OF THIS CASE								
SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:								
TOTAL NO. OF STEPS -		232						
TOTAL NO. OF DERIVATIVE EVALUATIONS -		349						
TOTAL NO. OF JACOBIAN EVALUATIONS -		41						
TOTAL CPU TIME -		1.460007 S						
TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 2.680008 S								
(LSEHS) READ DATA FOR NEXT CASE								

TABLE D.2.—Continued.

(o) Case 15

DISTANCE-AREA VERSION			LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM					NASA LEWIS RESEARCH CENTER		
LSENS METHANE AIR MECHAN. MON. DECR. TABULAR AREA WITH APRINT			CASE 15							
REACTION NUMBER	REACTION			REACTION RATE VARIABLES			ACTIVATION ENERGY			
				A	N					
1	M	+	1*CH4	=	1*CH3	+	1*H	2.00000E+17	0.0000	88000.00
2	1*H	+	1*CH4	=	1*CH3	+	1*H2	1.26000E+14	0.0000	11900.00
3	1*CH4	+	1*O2	=	1*CH3	+	1*HO2	7.94000E+13	0.0000	56000.00
4	1*O	+	1*CH4	=	1*CH3	+	1*OH	1.90000E+14	0.0000	11720.00
5	1*OH	+	1*CH4	=	1*CH3	+	1*H2O	2.50000E+13	0.0000	5010.00
6	1*CH3	+	1*O2	=	1*CH3O	+	1*O	2.40000E+13	0.0000	28680.00
7	1*CH3	+	1*OH	=	1*CH3O	+	1*H	6.30000E+12	0.0000	0.00
8	M	+	1*CH3O	=	1*CH2O	+	1*H	5.00000E+13	0.0000	21000.00
9			2*CH3	=	1*CH2H	+		2.40000E+14	-0.4000	0.00
10	1*H	+	1*CH2H	=	1*CH2	+	1*H2	1.32000E+14	0.0000	9700.00
11	1*O	+	1*CH2H	=	1*CH2	+	1*OH	1.13000E+14	0.0000	7850.00
12	1*OH	+	1*CH2H	=	1*CH2	+	1*H2O	8.70000E+13	0.0000	3520.00
13	M	+	1*CH2H	=	1*CH2H	+	1*H	1.00000E+17	0.0000	31000.00
14	1*CH2H	+	1*O2	=	1*CH2H	+	1*HO2	2.00000E+12	0.0000	5000.00
15	1*H	+	1*CH2H	=	1*CH2H	+	1*H2	4.80000E+13	0.0000	0.00
16	1*CH3	+	1*CH2H	=	1*CH2H	+	1*H	2.00000E+13	0.0000	0.00
17	1*H	+	1*CH2H	=	1*CH2H	+	1*CH2H	1.50000E+14	0.0000	10200.00
18	M	+	1*CH2H	=	1*CH2H	+	1*H2	2.60000E+17	0.0000	79300.00
19	1*CH2H	+	1*OH	=	1*CH2H	+	1*H2O	4.80000E+12	0.0000	1250.00
20	1*CH2H	+	1*OH	=	1*CH3	+	1*CH2O	2.00000E+12	0.0000	960.00
21	1*CH2H	+	1*O	=	1*CH3	+	1*HCO	3.30000E+12	0.0000	1150.00
22	1*CH2H	+	1*O	=	1*CH2O	+	1*CH2	2.50000E+13	0.0000	5000.00
23	M	+	1*CH2H	=	1*CH2H	+	1*H	3.00000E+15	0.0000	32000.00
24	1*CH2H	+	1*O2	=	1*CH2O	+	1*HCO	3.98000E+12	0.0000	-250.00
25	1*CH2H	+	1*H	=	1*CH2H	+	1*H2	6.00000E+12	0.0000	0.00
26	1*CH2H	+	1*O	=	1*CH2H2O	+	1*H	3.30000E+13	0.0000	0.00
27	1*CH2H	+	1*OH	=	1*CH2H	+	1*H2O	5.00000E+12	0.0000	0.00
28	1*CH2H	+	1*CH2	=	1*CH2H	+	1*CH3	3.00000E+13	0.0000	0.00
29	1*CH2H	+	1*CH2H	=	2*CH2H	+		0.0000E+13	0.0000	0.00
30	M	+	1*CH2H	=	1*CH2H	+	1*H	3.00000E+13	0.0000	107000.00
31	1*CH2H	+	1*O	=	1*CH2	+	1*CO	4.20000E+16	0.0000	9890.00
32	1*CH2H	+	1*O	=	1*CH2H	+	1*H	4.00000E+14	0.0000	10660.00
33	1*CH2H	+	1*OH	=	1*CH2H	+	1*H2O	6.30000E+12	0.0000	7000.00
34	1*CH2H	+	1*OH	=	1*CH2H2O	+	1*H	3.20000E+11	0.0000	200.00
35	1*CH2H	+	1*O2	=	1*CH2H	+	1*O	5.00000E+13	0.0000	1500.00
36	1*CH2H	+	1*OH	=	1*CH2H	+	1*H	2.00000E+13	0.0000	0.00
37	1*CH2H	+	1*O2	=	2*CO	+	1*OH	1.46000E+12	0.0000	2500.00
38	1*CH2H	+	1*O	=	2*CO	+	1*H	1.20200E+12	0.0000	0.00
39	1*CH2H	+	1*OH	=	2*HCO	+		1.00000E+13	0.0000	0.00
40	1*CH2H	+	1*H	=	1*CH2	+	1*CO	5.00000E+13	0.0000	0.00
41	1*CH2H	+	1*CH2	=	1*CH2H	+	1*CO	3.00000E+13	0.0000	0.00
42	1*CH2H	+	1*CH2	=	1*CH2O	+	1*CH2H	1.00000E+13	0.0000	2000.00
43			2*CH2H	=	1*CH2H	+	2*CO	1.00000E+13	0.0000	0.00
44	1*CH2H2O	+	1*OH	=	1*CH2O	+	1*HCO	2.80000E+13	0.0000	0.00
45	1*CH2H2O	+	1*OH	=	1*CH2H	+	1*H2O	7.50000E+12	0.0000	3000.00
46	1*CH2H2O	+	1*H	=	1*CH3	+	1*CO	1.13000E+13	0.0000	3428.00
47	1*CH2H2O	+	1*H	=	1*CH2H	+	1*H2	7.50000E+13	0.0000	8000.00
48	1*CH2H2O	+	1*O	=	1*CH2H	+	1*OH	5.00000E+13	0.0000	8000.00
49	1*CH2H2O	+	1*O	=	1*CH2O	+	1*CO	2.00000E+13	0.0000	0.00
50	H	+	1*CH2H2O	=	1*CH2	+	1*CO	2.00000E+16	0.0000	60000.00
51	1*CH2H	+	1*O	=	1*CO	+	1*CH	5.00000E+13	0.0000	0.00
52	1*CH3O	+	1*H2	=	1*CH2O	+	1*HO2	1.00000E+13	0.0000	7170.00
53	1*CH3O	+	1*H	=	1*CH2O	+	1*H2	2.00000E+13	0.0000	0.00
54	M	+	1*CH2O	=	1*HCO	+	1*H	5.00000E+16	0.0000	81000.00
55	1*CH2O	+	1*OH	=	1*HCO	+	1*H2O	3.00000E+13	0.0000	1200.00
56	1*CH2O	+	1*H	=	1*HCO	+	1*H2	2.50000E+13	0.0000	3990.00
57	1*CH2O	+	1*O	=	1*HCO	+	1*OH	3.50000E+13	0.0000	3510.00
58	1*CH3	+	1*CH2O	=	1*CH4	+	1*HCO	1.00000E+10	0.5000	6000.00
59	1*CH3	+	1*HCO	=	1*CH4	+	1*CO	3.00000E+11	0.5000	0.00
60	1*CH3	+	1*HO2	=	1*CH3O	+	1*OH	2.00000E+13	0.0000	0.00
61	M	+	1*CH3	=	1*CH2	+	1*H	1.95000E+16	0.0000	91600.00
62	1*H	+	1*CH3	=	1*H2	+	1*CH2	2.70000E+11	0.6700	25700.00
63	1*O	+	1*CH3	=	1*OH	+	1*CH2	1.90000E+11	0.6800	25700.00
64	1*OH	+	1*CH3	=	1*H2O	+	1*CH2	2.70000E+11	0.6700	25700.00
65	1*CH	+	1*CO2	=	1*HCO	+	1*CO	3.70000E+12	0.0000	0.00
66	1*CH	+	1*O2	=	1*HCO	+	1*O	1.00000E+13	0.0000	0.00
67	1*CH2	+	1*O2	=	1*CH2O	+	1*O	5.00000E+11	0.5000	6760.00
68	1*CH2	+	1*O	=	1*CH	+	1*OH	2.00000E+11	0.7000	25800.00
69	1*CH2	+	1*OH	=	1*CH	+	1*H2O	5.00000E+11	0.5000	5900.00
70	1*CH2	+	1*H	=	1*CH	+	1*H2	3.20000E+11	0.7000	4970.00
71			2*CH2	=	1*CH2H	+	1*H	5.00000E+12	0.0000	0.00
72			2*CH2	=	1*CH2H	+	1*H2	4.00000E+13	0.0000	0.00
73	1*HCO	+	1*O2	=	1*CO	+	1*HO2	3.00000E+13	0.0000	0.00
74	1*HCO	+	1*O	=	1*CO	+	1*OH	3.00000E+13	0.0000	0.00
75	1*HCO	+	1*OH	=	1*CO	+	1*H2O	3.00000E+13	0.0000	0.00
76	1*HCO	+	1*H	=	1*CO	+	1*H2	2.00000E+13	0.0000	0.00
77	M	+	1*HCO	=	1*H	+	1*CO	2.90000E+14	0.0000	15570.00
78	1*CO	+	1*O	=	1*CO2	+	M	2.40000E+15	0.0000	4100.00
79	1*CO	+	1*O2	=	1*CO2	+	1*O	2.50000E+12	0.0000	47490.00
80	1*CO	+	1*OH	=	1*CO2	+	1*H	4.17000E+11	0.0000	1000.00
81	1*CO	+	1*HO2	=	1*CO2	+	1*OH	5.75000E+13	0.0000	22950.00
82	1*O	+	1*H2O	=	2*OH	+		6.80000E+13	0.0000	18365.00
83	1*H	+	1*O2	=	1*OH	+	1*O	1.89000E+14	0.0000	16400.00
84	1*H	+	1*H2	=	1*OH	+	1*H	4.20000E+14	0.0000	15750.00
85	1*H	+	1*HO2	=	1*H2	+	1*O2	7.28000E+13	0.0000	2126.00
86	1*O	+	1*HO2	=	1*OH	+	1*O2	5.00000E+13	0.0000	1000.00
87	1*HO2	+	1*OH	=	1*H2O	+	1*O2	8.00000E+12	0.0000	0.00
88	1*H	+	1*HO2	=	2*OH	+		1.34000E+14	0.0000	1070.00
89	1*H2	+	1*HO2	=	1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00
90	1*OH	+	1*H2O2	=	1*H2O	+	1*HO2	6.10000E+12	0.0000	1450.00
91			2*HO2	=	1*H2O2	+	1*O2	1.80000E+12	0.0000	0.00
92	1*H	+	1*H2O2	=	1*OH	+	1*H2O	7.80000E+11	0.0000	0.00
93	M	+	1*H2O2	=	2*OH	+		1.44000E+17	0.0000	45510.00
94	1*H2	+	1*OH	=	1*H2O	+	1*H	4.74000E+13	0.0000	6098.00
95	1*H	+	1*O2	=	1*HO2	+	M	1.46000E+15	0.0000	1000.00
96	H	+	1*H2O	=	1*H	+	1*OH	1.30000E+15	0.0000	105140.00
97	1*H	+	1*O	=	1*OH	+	M	7.10000E+18	1.0000	0.00
98	M	+	1*H2	=	2*H	+		2.20000E+14	0.0000	76000.00
99	H	+	1*O2	=	2*O	+		1.80000E+18	-1.0000	118020.00
100	1*CH	+	1*H2	=	1*HCN	+	1*H	1.00000E+11	0.0000	19000.00
101	1*CN	+	1*H2	=	1*HCN	+	1*H	6.00000E+13	0.0000	5500.00
102	1*O	+	1*HCN	=	1*OH	+	1*CN	1.40000E+11	0.6800	16700.00
103	1*OH	+	1*HCN	=	1*HNC	+	1*H	4.00000E+11	0.0000	2800.00
104	1*H	+	1*O	=	1*CO	+	1*H	1.20000E+13	0.0000	0.00

TABLE D.2.—Continued.
(c) Continued.

105	1*H	+	1*OH	=	1*HCO	+	1*H	2.50000E+14	0.0000	6000.00
106	1*H2	+	1*HCO	=	1*HHCO	+	1*H	1.00000E+14	0.0000	9000.00
107	1*HHCO	+	1*H	=	1*HH2	+	1*CO	1.00000E+14	0.0000	8500.00
108	1*H	+	1*G2	=	1*HCO	+	1*O	3.20000E+13	0.0000	1000.00
109	1*H	+	1*CO2	=	1*HCO	+	1*CO	3.70000E+12	0.0000	0.00
110	1*O	+	1*HCO	=	1*HO	+	1*CO	2.00000E+13	0.0000	0.00
111	1*H	+	1*HCO	=	1*H2	+	1*CO	1.00000E+13	0.0000	0.00
112	1*H	+	1*HCO	=	1*HH	+	1*CO	2.00000E+13	0.0000	0.00
113	1*CH	+	1*HO	=	1*H	+	1*HCO	1.60000E+13	0.0000	9940.00
114	1*CH	+	1*HO	=	1*O	+	1*HCN	2.00000E+12	0.0000	0.00
115	1*HH	+	1*OH	=	1*H	+	1*H2O	5.00000E+11	0.5000	2000.00
116	1*HO2	+	1*HO	=	1*HO2	+	1*OH	2.09000E+12	0.0000	-477.00
117	1*O	+	1*HO2	=	1*HO	+	1*O2	1.00000E+13	0.0000	596.00
118	1*HO	+	1*O	=	1*HO2	+	M	5.62000E+15	0.0000	-1160.00
119	1*HO2	+	1*H	=	1*HO	+	1*OH	3.47000E+14	0.0000	1470.00
120	1*HO	+	1*H	=	1*H	+	1*OH	2.63000E+14	0.0000	50410.00
121	1*HO	+	1*O	=	1*H	+	1*O2	3.80000E+09	1.0000	41370.00
122	1*O	+	1*H2	=	1*HO	+	1*H	1.80000E+14	0.0000	76250.00
123	1*H	+	1*HO2	=	2*HO	+	1*O	4.00000E+12	0.0000	0.00
124	M	+	1*H2O	=	1*H2	+	1*O	6.92000E+23	-2.5000	65000.00
125	1*O	+	1*H2O	=	1*H2	+	1*O2	1.00000E+14	0.0000	28020.00
126	1*O	+	1*H2O	=	2*HO	+	1*O	6.92000E+13	0.0000	26630.00
127	1*H2O	+	1*H	=	1*H2	+	1*OH	7.59000E+13	0.0000	15100.00
128	1*HO2	+	1*H2	=	1*HHO2	+	1*H	2.40000E+13	0.0000	29000.00
129	1*OH	+	1*HO2	=	1*HHO3	+	M	3.00000E+15	0.0000	-3800.00
130	1*OH	+	1*HO	=	1*HHO2	+	M	5.60000E+15	0.0000	-1700.00
131	1*HHO	+	1*H	=	1*H2	+	1*NO	5.00000E+12	0.0000	0.00
132	1*H	+	1*HO	=	1*HHO	+	M	5.40000E+15	0.0000	-600.00
133	1*HHO	+	1*OH	=	1*H2O	+	1*HO	3.60000E+13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	, 93) = 2.30000	M(O2	, 93) = 0.78000	M(H2O	, 93) = 6.00000	M(H2O2	, 93) = 6.60000
M(O2	, 95) = 1.30000	M(H2	, 95) = 1.30000	M(H2O	, 95) = 21.30000	M(CO2	, 95) = 7.00000
M(H2	, 96) = 4.00000	M(O2	, 96) = 1.50000	M(H2O	, 96) = 20.00000	M(H2	, 96) = 1.50000
M(CO2	, 96) = 4.00000	M(H2	, 98) = 4.10000	M(O2	, 98) = 2.00000	M(H2O	, 98) = 15.00000
M(H2	, 98) = 2.00000	M(O2	, 129) = 0.70000	M(H2	, 129) = 1.40000		

** HEH INPUT DATA GIVEN IN CGS UNITS **

** OUTPUT REQUIRED IN CGS UNITS **

** ASSIGNED VARIABLE PROFILE **

THE AREA IS CALCULATED BY INTERPOLATION FROM THE FOLLOWING TABLE

STATION	AXIAL DISTANCE (CM)	AREA (CM**2)
1	0.00000E+00	1.20000E+03
2	5.00000E+00	1.18000E+03
3	1.00000E+01	1.16000E+03
4	1.50000E+01	1.14000E+03
5	2.00000E+01	1.12000E+03
6	2.50000E+01	1.10000E+03
7	3.00000E+01	1.08000E+03
8	3.20000E+01	1.06000E+03
9	3.40000E+01	1.04000E+03
10	3.60000E+01	1.02000E+03
11	3.80000E+01	1.00000E+03
12	4.00000E+01	9.80000E+02
13	4.20000E+01	9.60000E+02
14	4.40000E+01	9.40000E+02

NUMBER OF REACTING SPECIES: 39

NUMBER OF INERT SPECIES: 0

NUMBER OF SPECIES ODE'S REQUIRED FOR THIS CASE: 39

TOTAL NUMBER OF ODE'S REQUIRED FOR THIS CASE: 42

INTEGRATION CONTROLS

INTEGRATION METHOD (MF): 21 MAXIMUM RELATIVE ERROR: 1.00000E-05 SPECIES ABSOLUTE ERROR: 1.00000E-14

MAXIMUM NUMBER OF STEPS ALLOWED FOR THE COMPLETE PROBLEM: 2000

** OUTPUT REQUIRED AT 4 ASSIGNED-VARIABLE VALUES WHICH CORRESPOND TO THE FOLLOWING PRINT STATIONS **

STATION	AXIAL DISTANCE (CM)
1	5.00000E+00
2	1.24954E+01
3	2.24363E+01
4	4.30002E+01

TABLE D.2.—Continued.
(c) Continued.

** INITIAL CONDITIONS **									
TIME	0.00000E+00	SEC	AREA	1.20000E+03	SQ CM	AXIAL POSITION	0.00000E+00	CM	
FLOW PROPERTIES					INTEGRATION INDICATORS				
PRESSURE (ATM)	1.73000		STEPS FROM LAST PRINT	0					
VELOCITY (CM/SEC)	155259.65		AVERAGE STEP SIZE	0.00000E+00					
DENSITY (G/CM**3)	3.71736E-04		METHOD ORDER	0					
TEMPERATURE (DEG K)	1600.00								
MASS FLOW RATE (G/SEC)	6.92587E+04		TOTAL NUMBER OF STEPS	0					
ENTROPY (CAL/G/DEG K)	2.1223		FUNCT EVALUATIONS	0					
MACH NUMBER	2.0000		JACOBIAN EVALUATIONS	0					
GAMMA	1.2780								
ENTHALPY (CAL/G)	3.46688E+02								
SP. HEAT (CP) (CAL/G/DEG K)	3.23820E-01								
CHEMICAL PROPERTIES									
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST COS UNITS	NET REACTION CONV RATE (MOLE/CM**3/G**2/SEC)	NET RATE/POSITIONAL DIR RATE		
CH4	6.55792E-07	4.97680E-02	-4.71274E-06	1	1.9089E+05	1.19373E+01	1.00000		
CH3	0.00000E+00	0.00000E+00	4.71274E-06	2	2.9847E+12	0.00000E+00	0.00000		
H	0.00000E+00	0.00000E+00	1.64958E-06	3	1.7806E+06	2.21667E+01	1.00000		
H2	0.00000E+00	0.00000E+00	0.00000E+00	4	4.7630E+12	0.00000E+00	0.00000		
O2	2.62317E-06	1.99072E-01	-8.38235E-05	5	5.1714E+12	0.00000E+00	0.00000		
H2O	0.00000E+00	0.00000E+00	3.06316E-06	6	2.9021E+09	0.00000E+00	0.00000		
O	0.00000E+00	0.00000E+00	8.07603E-05	7	6.3000E+12	0.00000E+00	0.00000		
OH	0.00000E+00	0.00000E+00	0.00000E+00	8	6.7687E+10	0.00000E+00	0.00000		
H2O	0.00000E+00	0.00000E+00	0.00000E+00	9	1.2548E+13	0.00000E+00	0.00000		
CH3O	0.00000E+00	0.00000E+00	0.00000E+00	10	6.2462E+12	0.00000E+00	0.00000		
CH2O	0.00000E+00	0.00000E+00	0.00000E+00	11	9.5679E+12	0.00000E+00	0.00000		
C2H6	0.00000E+00	0.00000E+00	0.00000E+00	12	2.8755E+13	0.00000E+00	0.00000		
C2H5	0.00000E+00	0.00000E+00	0.00000E+00	13	5.8291E+12	0.00000E+00	0.00000		
C2H4	0.00000E+00	0.00000E+00	0.00000E+00	14	4.1501E+11	0.00000E+00	0.00000		
CH2	0.00000E+00	0.00000E+00	0.00000E+00	15	4.8000E+13	0.00000E+00	0.00000		
C2H5	0.00000E+00	0.00000E+00	0.00000E+00	16	2.0000E+13	0.00000E+00	0.00000		
C2H2	0.00000E+00	0.00000E+00	0.00000E+00	17	6.0651E+12	0.00000E+00	0.00000		
HCO	0.00000E+00	0.00000E+00	0.00000E+00	18	5.8291E+06	0.00000E+00	0.00000		
C2H2O	0.00000E+00	0.00000E+00	0.00000E+00	19	3.2601E+12	0.00000E+00	0.00000		
C2H	0.00000E+00	0.00000E+00	0.00000E+00	20	1.4788E+12	0.00000E+00	0.00000		
CO	0.00000E+00	0.00000E+00	0.00000E+00	21	2.3129E+12	0.00000E+00	0.00000		
C2HO	0.00000E+00	0.00000E+00	0.00000E+00	22	5.1877E+12	0.00000E+00	0.00000		
CH	0.00000E+00	0.00000E+00	0.00000E+00	23	1.2768E+11	0.00000E+00	0.00000		
CO2	0.00000E+00	0.00000E+00	0.00000E+00	24	4.3056E+12	0.00000E+00	0.00000		
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	25	6.0000E+12	0.00000E+00	0.00000		
H2	9.89802E-06	7.51160E-01	-1.79633E-12	26	3.3000E+13	0.00000E+00	0.00000		
HCN	0.00000E+00	0.00000E+00	0.00000E+00	27	5.0000E+12	0.00000E+00	0.00000		
H	0.00000E+00	0.00000E+00	0.00000E+00	28	3.0000E+13	0.00000E+00	0.00000		
CH	1.31770E-12	1.00000E-07	-8.07603E-05	29	3.0000E+13	0.00000E+00	0.00000		
HICO	0.00000E+00	0.00000E+00	0.00000E+00	30	1.0180E+02	0.00000E+00	0.00000		
HCN	0.00000E+00	0.00000E+00	8.07603E-05	31	7.1320E+12	0.00000E+00	0.00000		
H2	0.00000E+00	0.00000E+00	0.00000E+00	32	1.3995E+13	0.00000E+00	0.00000		
HO	0.00000E+00	0.00000E+00	0.00000E+00	33	5.9692E+11	0.00000E+00	0.00000		
NH	0.00000E+00	0.00000E+00	0.00000E+00	34	3.0049E+11	0.00000E+00	0.00000		
H2O	0.00000E+00	0.00000E+00	0.00000E+00	35	3.1195E+13	0.00000E+00	0.00000		
H2O	0.00000E+00	0.00000E+00	1.79633E-12	36	2.0000E+13	0.00000E+00	0.00000		
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	37	6.6507E+11	0.00000E+00	0.00000		
HNO2	0.00000E+00	0.00000E+00	0.00000E+00	38	1.2020E+12	0.00000E+00	0.00000		
HNO3	0.00000E+00	0.00000E+00	0.00000E+00	39	1.0000E+13	0.00000E+00	0.00000		
HNO	0.00000E+00	0.00000E+00	0.00000E+00	40	5.0000E+13	0.00000E+00	0.00000		
				41	3.0000E+13	0.00000E+00	0.00000		
				42	5.3311E+12	0.00000E+00	0.00000		
				43	1.0000E+13	0.00000E+00	0.00000		
				44	2.8000E+13	0.00000E+00	0.00000		
				45	2.9193E+12	0.00000E+00	0.00000		
				46	3.8465E+12	0.00000E+00	0.00000		
				47	6.0578E+12	0.00000E+00	0.00000		
				48	4.0385E+12	0.00000E+00	0.00000		
				49	2.0000E+13	0.00000E+00	0.00000		
				50	1.2747E+08	0.00000E+00	0.00000		
				51	5.0000E+13	0.00000E+00	0.00000		
				52	1.0486E+12	0.00000E+00	0.00000		
				53	2.0000E+13	0.00000E+00	0.00000		
				54	4.3141E+05	0.00000E+00	0.00000		
				55	2.0569E+13	0.00000E+00	0.00000		
				56	7.1276E+12	0.00000E+00	0.00000		
				57	1.1604E+13	0.00000E+00	0.00000		
				58	6.0604E+10	0.00000E+00	0.00000		
				59	1.2000E+13	0.00000E+00	0.00000		
				60	2.0000E+13	0.00000E+00	0.00000		
				61	5.9987E+03	0.00000E+00	0.00000		
				62	1.1686E+10	0.00000E+00	0.00000		
				63	8.8532E+09	0.00000E+00	0.00000		
				64	1.1686E+10	0.00000E+00	0.00000		
				65	3.7000E+12	0.00000E+00	0.00000		
				66	1.0000E+13	0.00000E+00	0.00000		
				67	2.2405E+12	0.00000E+00	0.00000		
				68	1.0466E+10	0.00000E+00	0.00000		
				69	3.1270E+12	0.00000E+00	0.00000		
				70	1.1726E+13	0.00000E+00	0.00000		
				71	5.0000E+12	0.00000E+00	0.00000		
				72	4.0000E+13	0.00000E+00	0.00000		
				73	3.0000E+13	0.00000E+00	0.00000		
				74	5.0000E+13	0.00000E+00	0.00000		
				75	3.0000E+13	0.00000E+00	0.00000		
				76	2.0000E+13	0.00000E+00	0.00000		
				77	2.1659E+12	0.00000E+00	0.00000		
				78	6.6096E+14	0.00000E+00	0.00000		
				79	7.6523E+05	0.00000E+00	0.00000		
				80	3.0447E+11	0.00000E+00	0.00000		
				81	4.2421E+10	0.00000E+00	0.00000		
				82	2.1085E+11	0.00000E+00	0.00000		
				83	1.0872E+12	0.00000E+00	0.00000		
				84	5.3603E+12	0.00000E+00	0.00000		
				85	3.7302E+13	0.00000E+00	0.00000		

TABLE D.2.—Continued.
(c) Continued.

86	3.6507E+13	0.00000E+00	0.00000
87	8.0000E+12	0.00000E+00	0.00000
88	9.5708E+13	0.00000E+00	0.00000
89	3.0432E+10	0.00000E+00	0.00000
90	3.8905E+12	0.00000E+00	0.00000
91	1.8000E+12	0.00000E+00	0.00000
92	7.8000E+11	0.00000E+00	0.00000
93	8.7496E+10	0.00000E+00	0.00000
94	6.9635E+12	0.00000E+00	0.00000
95	1.9996E+15	0.00000E+00	0.00000
96	5.6558E+00	0.00000E+00	0.00000
97	4.4375E+15	0.00000E+00	0.00000
98	1.6960E+01	0.00000E+00	0.00000
99	8.5187E-02	2.1308E-05	1.00000
100	2.5393E+08	0.00000E+00	0.00000
101	1.1329E+13	0.00000E+00	0.00000
102	1.0387E+11	0.00000E+00	0.00000
103	1.6581E+11	0.00000E+00	0.00000
104	1.2000E+13	0.00000E+00	0.00000
105	3.7877E+13	0.00000E+00	0.00000
106	5.8974E+12	0.00000E+00	0.00000
107	6.9017E+12	0.00000E+00	0.00000
108	2.3364E+13	5.84425E+02	1.00000
109	3.7000E+12	0.00000E+00	0.00000
110	2.0000E+13	0.00000E+00	0.00000
111	1.0000E+13	0.00000E+00	0.00000
112	2.0000E+13	0.00000E+00	0.00000
113	7.0207E+11	0.00000E+00	0.00000
114	2.0000E+12	0.00000E+00	0.00000
115	1.0662E+13	0.00000E+00	0.00000
116	2.4283E+12	0.00000E+00	0.00000
117	8.2907E+12	0.00000E+00	0.00000
118	8.0946E+15	0.00000E+00	0.00000
119	2.1854E+14	0.00000E+00	0.00000
120	3.4219E+07	0.00000E+00	0.00000
121	1.3584E+07	0.00000E+00	0.00000
122	6.9185E+03	0.00000E+00	0.00000
123	4.0000E+12	0.00000E+00	0.00000
124	8.9376E+06	0.00000E+00	0.00000
125	1.4882E+10	-1.29992E-05	1.00000
126	1.5945E+10	0.00000E+00	0.00000
127	6.5717E+11	0.00000E+00	0.00000
128	2.6242E+09	0.00000E+00	0.00000
129	9.9124E+15	0.00000E+00	0.00000
130	9.5587E+15	0.00000E+00	0.00000
131	5.0000E+12	0.00000E+00	0.00000
132	6.5215E+15	0.00000E+00	0.00000
133	3.6000E+13	0.00000E+00	0.00000

DERIVATIVES (CGS UNITS): T 1.97928E+00 RHO 1.65526E-06 V -1.72834E-02
MIXTURE MOLECULAR HEIGHT 28.21102 TOTAL ENERGY EXCHANGE RATE -1.27744E+06 MASS FRACTION SUM 1.00000000
(CAL-CM**3/G**2/SEC)

CPU TIME FOR INITIALIZATION OF LSENS = 2.220001 5

TIME 1.46451E-04 SEC AREA 1.10936E+03 SQ CM AXIAL POSITION 2.24363E+01 CM

FLOW PROPERTIES

PRESSURE 1.98504
(ATM)
VELOCITY 150959.76
(CM/SEC)
DENSITY 4.13563E-04
(G/CM**3)
TEMPERATURE 1650.17
(DEG K)
MASS FLOW RATE 6.92587E+04
(G/SEC)
ENTROPY 2.1234
(CAL/G/DEG K)
MACH NUMBER 1.9161
GAMMA 1.2763
ENTHALPY 3.62423E+02
(CAL/G)
SP. HEAT (CP) 3.25371E-01
(CAL/G/DEG K)

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 29
AVERAGE STEP SIZE 0.35712E+00
METHOD ORDER 4
TOTAL NUMBER OF STEPS 161
FUNCT EVALUATIONS 199
JACOBIAN EVALUATIONS 25

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POST- TIVE DIR RATE
CH4	7.17624E-07	4.89515E-02	-2.51430E-04	1	4.4284E+05	2.65382E+01	0.97428
CH3	3.70822E-09	2.52950E-04	5.03006E-05	2	3.3445E+12	9.58538E+01	0.97496
H	7.00621E-12	4.77918E-07	1.25105E-07	3	3.0419E+06	2.82779E+01	0.76098
H2	7.91112E-10	5.39645E-05	-1.66017E-05	4	5.3278E+12	3.79712E+02	0.99957
O2	2.91153E-06	1.98605E-01	-1.46771E-04	5	5.4252E+12	9.45846E+02	0.99824
HO2	9.44564E-10	6.44319E-05	7.30120E-06	6	3.8178E+09	2.40782E+02	0.99910
O	1.69934E-11	1.15917E-06	2.71685E-07	7	4.3000E+12	-9.40230E+00	0.62316
OH	4.16255E-11	2.83942E-06	7.69567E-07	8	8.2740E+10	1.72728E+02	1.00000
H2O	7.12085E-09	4.85737E-04	1.68311E-04	9	1.2394E+13	2.67191E+02	0.26815
CH3O	2.43557E-11	1.66139E-06	4.42876E-07	10	6.8533E+12	5.08339E-01	1.00000
CH2O	4.35616E-09	2.97148E-04	1.03105E-04	11	1.0314E+13	1.85554E+00	1.00000
C2H6	1.81074E-09	1.23516E-04	4.30530E-05	12	2.9739E+13	1.31057E+01	1.00000
C2H5	2.28401E-14	1.55800E-09	7.69219E-10	13	7.8404E+12	1.53007E+01	0.99685
C2H4	5.74154E-11	3.91650E-06	2.72323E-06	14	4.3534E+11	1.64508E-01	0.97073
CH2	1.33148E-15	9.08247E-11	6.47922E-11	15	4.8000E+13	4.47719E-05	0.99693
C2H5	6.99639E-16	4.77248E-11	4.59942E-11	16	2.0000E+13	5.72222E-04	0.99976
C2H2	1.40319E-13	9.57162E-09	8.59543E-09	17	6.6865E+12	1.57259E-02	0.99998
HCO	4.83642E-14	3.29909E-09	1.94512E-09	18	8.1738E+06	4.02252E-02	1.00000
C2H2O	3.63527E-16	2.47974E-11	2.56029E-11	19	3.2987E+12	4.60939E-02	1.00000
C2H	4.71926E-20	3.21916E-15	3.95994E-15	20	1.4924E+12	-6.02946E-01	0.96657

TABLE D.2.—Continued.

(o) Continued.

CO	1.30390E-10	8.89436E-06	6.00063E-06	21	2.3381E+12	1.33377E-02	1.00000
C2H6	2.00636E-17	1.36860E-12	1.57301E-12	22	5.4417E+12	3.10425E-02	0.99998
CH	1.04070E-20	7.09898E-16	7.22928E-16	23	1.7339E+11	1.03905E-02	0.99930
CO2	1.42213E-13	9.70085E-09	8.80828E-09	24	4.2953E+12	5.11571E-02	1.00000
H2O2	8.54763E-13	5.83063E-08	1.03216E-08	25	6.0000E+12	1.71843E-07	0.99932
H2	1.10117E-05	7.51146E-01	-9.52715E-11	26	3.3000E+13	2.29396E-06	1.00000
HCl	4.10903E-18	2.80291E-13	1.90069E-13	27	5.0000E+12	8.51335E-07	0.99995
N	1.46099E-18	9.96594E-14	4.38093E-14	28	3.0000E+13	-3.29911E-09	0.95281
CH	5.12271E-18	3.49437E-13	1.22903E-13	29	3.0000E+13	4.32687E-15	0.74712
HNCO	2.59465E-13	1.76990E-08	5.95718E-09	30	2.8320E+02	3.39666E-09	0.99724
NO	1.17461E-12	8.01242E-08	-6.53491E-09	31	7.8396E+12	1.09293E-04	1.00000
H2	2.97443E-16	2.02896E-11	1.36082E-11	32	1.5697E+13	2.16050E-04	1.00000
NO	2.14401E-14	1.46250E-09	3.66046E-10	33	7.4517E+11	2.54429E-05	0.99981
HM	8.96606E-15	6.11605E-10	1.60472E-10	34	3.0107E+11	1.02814E-05	0.99999
NO2	1.38841E-15	9.47083E-11	4.26103E-11	35	3.1645E+13	2.54226E-05	1.00000
N2O	4.48392E-15	3.05864E-10	9.25858E-11	36	2.0000E+13	2.29331E-10	0.99835
HNO2	1.76860E-20	1.20643E-15	5.84728E-16	37	6.8116E+11	2.32647E-04	1.00000
HNO3	1.71978E-22	1.17312E-17	7.01640E-18	38	1.2020E+12	2.39612E-09	1.00000
HNO	6.02737E-20	4.11148E-15	1.98166E-15	39	1.0000E+13	4.88248E-08	0.99990
				40	5.0000E+13	3.98351E-08	0.96936
				41	3.0000E+13	4.68574E-12	0.99999
				42	5.4340E+12	2.84658E-12	0.77032
				43	1.0000E+13	2.35361E-16	1.00000
				44	2.8000E+13	-1.17593E-04	0.97937
				45	3.0043E+12	2.56633E-07	0.96552
				46	3.9726E+12	-2.76520E-05	0.99787
				47	6.5394E+12	4.95944E-08	0.50928
				48	4.3596E+12	1.56133E-07	0.99156
				49	2.0000E+13	7.22375E-07	1.00000
				50	2.2625E+08	6.94081E-06	0.98456
				51	5.0000E+13	2.34445E-10	1.00000
				52	1.1231E+12	4.65627E+02	1.00000
				53	2.0000E+13	1.99941E-02	1.00000
				54	9.3599E+05	3.49479E-01	1.00000
				55	2.0806E+13	2.20583E+01	1.00000
				56	7.4046E+12	1.32131E+00	1.00000
				57	1.2001E+13	5.19399E+00	1.00000
				58	6.5181E+10	6.15586E+00	0.99996
				59	1.2187E+13	1.27777E-02	0.99991
				60	2.0000E+13	4.09585E+02	1.00000
				61	1.4403E+04	4.57785E-03	0.99997
				62	1.5254E+10	2.31704E-03	0.99997
				63	1.1560E+10	4.25900E-03	1.00000
				64	1.5254E+10	1.37665E-02	1.00000
				65	3.7000E+12	-5.25069E-13	0.14089
				66	1.0000E+13	1.77160E-06	1.00000
				67	2.4319E+12	5.51211E-02	1.00000
				68	1.3688E+10	1.81077E-09	1.00000
				69	5.3600E+12	1.08877E-06	0.99978
				70	1.2564E+13	6.85206E-07	0.99976
				71	5.0000E+12	5.18176E-11	0.99982
				72	4.0000E+13	4.14616E-10	1.00000
				73	3.0000E+13	2.46987E+01	0.99998
				74	3.0000E+13	1.44159E-04	1.00000
				75	3.0000E+13	3.53120E-04	1.00000
				76	2.0000E+13	3.96236E-05	1.00000
				77	2.5136E+12	1.04200E+01	1.00000
				78	6.8739E+14	1.30550E-04	1.00000
				79	1.2074E+06	2.67993E-03	1.00000
				80	3.0739E+11	9.75451E-03	0.99997
				81	5.2820E+10	3.80361E-02	1.00000
				82	2.5132E+11	1.34282E-01	0.75519
				83	1.2718E+12	1.51638E+02	0.99966
				84	6.3415E+12	4.89877E-01	0.98280
				85	3.8068E+13	1.31865E+00	0.89523
				86	3.6858E+13	3.45287E+00	0.99820
				87	5.0000E+12	1.82553E+00	0.99264
				88	3.6693E+13	5.74132E+00	1.00000
				89	3.8651E+10	1.67619E-01	0.99261
				90	3.9440E+12	-6.97878E-03	0.85480
				91	1.8000E+12	9.38243E+00	0.99923
				92	7.8000E+11	2.73111E-05	0.99999
				93	1.3520E+11	9.49668E+00	0.99942
				94	7.3817E+12	1.32137E+00	0.92973
				95	1.9806E+15	-3.71788E+01	0.89238
				96	1.5457E+01	-1.90679E-04	0.93159
				97	4.3026E+15	4.31723E-05	0.98325
				98	4.2473E+01	-1.53311E-07	0.02648
				99	2.5532E-01	6.24295E-05	0.97979
				100	3.0453E+08	2.04044E-10	1.00000
				101	1.1918E+13	2.82378E-07	0.99991
				102	1.2468E+11	9.51698E-09	0.99468
				103	1.7030E+11	-8.19194E-07	0.99979
				104	1.2000E+13	6.10770E-09	1.00000
				105	4.0114E+13	7.76301E-05	0.99936
				106	6.4274E+12	3.49108E-02	0.99972
				107	7.4861E+12	7.95644E-05	0.99997
				108	2.3589E+13	9.75761E-04	0.47435
				109	3.7000E+12	8.99142E-04	1.00000
				110	2.0000E+13	2.33411E-03	1.00000
				111	1.0000E+13	1.00337E-10	1.00000
				112	2.0000E+13	9.62332E-04	1.00000
				113	7.7207E+11	9.97601E-16	0.99044
				114	2.0000E+12	2.60178E-15	0.99717
				115	1.1033E+13	2.40839E-05	0.99999
				116	2.4172E+12	2.85250E-04	0.99662
				117	8.3381E+12	5.36739E-07	0.46681
				118	8.0051E+15	-2.29534E-05	0.98923
				119	2.2164E+14	1.26032E-05	0.99982
				120	5.5414E+07	-1.46332E-08	0.99669
				121	2.0808E+07	-3.95127E-05	1.00000
				122	1.4344E+04	1.56934E-05	1.00000
				123	4.0000E+12	4.74400E-14	1.00000
				124	1.5404E+07	-5.04319E-04	0.98840
				125	1.9454E+10	-3.69577E-05	0.99977
				126	2.0569E+10	9.16355E-09	1.00000
				127	7.5925E+11	-6.18438E-08	0.30722
				128	5.4628E+09	2.22342E-09	0.99981
				129	9.5586E+15	4.10234E-11	0.00092

TABLE D.2.—Continued.
(o) Continued.

			130	9.4045E+15	-1.88154E-08	0.02549
			131	5.0000E+12	-1.70434E-12	0.12131
			132	6.4842E+15	1.20705E-08	0.14458
			133	3.6000E+13	4.85855E-10	0.92002
DERIVATIVES (CGS UNITS): T	2.88791E+00	RHO	2.20037E-06	V	-2.27804E+02	
MIXTURE MOLECULAR HEIGHT	28.21051	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	-4.25939E+07	MASS FRACTION SUM	1.00000000	

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 1.649994E+00 S UP TO THIS TIME - 9.000000E+00 S

TIME	2.83463E-04 SEC	AREA	9.54999E+02 SQ CM	AXIAL POSITION	4.25001E+01 CM
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FLOW PROPERTIES

PRESSURE (ATM)	3.17523
VELOCITY (CM/SEC)	133515.05
DENSITY (G/CM**3)	5.43172E-04
TEMPERATURE (DEG K)	1993.74
MASS FLOW RATE (G/SEC)	6.92581E+04
ENTROPY (CAL/G/DEG K)	2.1774
MACH NUMBER	1.5379
GAMMA	1.2725
ENTHALPY (CAL/G)	4.21727E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.31576E-01

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	118
AVERAGE STEP SIZE	0.16567E+00
METHOD ORDER	4
TOTAL NUMBER OF STEPS	279
FUNCT EVALUATIONS	359
JACOBIAN EVALUATIONS	38

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSTIVE DIR RATE
CH4	3.40604E-07	1.75491E-02	-6.38759E-02	1	4.5147E+07	-2.98324E+03	0.74678
CH3	1.27900E-07	6.58980E-03	1.67191E-02	2	6.2505E+12	1.95450E+04	0.76983
H	3.51845E-09	1.81282E-04	1.43170E-03	3	5.7703E+07	-1.02029E+03	0.82067
H2	4.92214E-08	2.53605E-03	3.55775E-03	4	9.8634E+12	7.00746E+04	0.96748
O2	3.34688E-06	1.72442E-01	-6.64194E-02	5	7.0592E+12	1.34032E+05	0.93620
H2O	5.69348E-09	2.93347E-04	2.42905E-04	6	1.7233E+10	2.31976E+04	0.92778
O	6.36081E-09	3.27730E-04	2.81115E-03	7	6.3000E+12	-3.74404E+04	0.43831
OH	1.75676E-08	9.05141E-04	7.32808E-03	8	2.4945E+11	1.62448E+04	1.00000
H2O	6.74531E-07	3.47341E-02	8.94642E-02	9	1.1491E+13	6.62632E+04	0.10401
CH3O	9.89933E-10	5.10046E-05	6.96576E-05	10	1.1410E+13	3.96710E+03	0.99994
CH2O	5.29882E-08	2.73013E-03	-5.09769E-03	11	1.5580E+13	9.79384E+03	0.99999
C2H6	2.91571E-08	1.50227E-03	-2.83783E-03	12	3.5782E+13	6.21209E+03	0.99998
C2H5	3.55738E-11	1.83288E-06	8.32677E-06	13	3.9979E+13	7.56667E+04	0.80876
C2H4	7.70981E-08	3.97235E-03	7.73786E-03	14	5.6616E+11	1.66776E+02	0.72996
CH2	2.79446E-10	1.43980E-05	1.57683E-04	15	4.8000E+13	2.01363E+01	0.98885
C2H3	2.38724E-10	1.22998E-05	1.10005E-04	16	2.0000E+13	2.42156E+03	0.99948
C2H2	8.96820E-09	4.62071E-04	2.59896E-03	17	1.1428E+13	1.04976E+04	0.99904
HCO	1.53395E-10	7.90341E-06	4.93156E-05	18	5.2753E+08	2.67555E+03	0.99999
C2H2O	1.07069E-10	5.51652E-06	5.1763E-05	19	3.5189E+12	1.61502E+04	0.99973
C2H	1.44852E-12	7.46325E-08	1.08700E-06	20	1.5696E+12	6.83922E+03	0.94914
CO	1.98863E-07	1.02461E-02	3.46349E-02	21	2.4811E+12	4.12407E+03	1.00000
C2H2O	4.59648E-10	2.36826E-05	3.20739E-04	22	7.0770E+12	1.17617E+04	0.99986
CH	1.24851E-12	6.43273E-08	1.27908E-06	23	9.3184E+11	1.45445E+04	0.99390
CO2	4.31797E-09	2.22476E-04	1.35990E-03	24	4.2392E+12	1.14802E+04	1.00000
H2O2	4.15768E-12	2.14218E-07	4.19770E-07	25	6.0000E+12	1.70733E+01	0.99964
N2	1.44628E-05	7.45169E-01	-2.43752E-07	26	3.3000E+13	1.69843E+02	1.00000
HCN	2.20298E-14	1.13505E-09	1.56265E-08	27	5.0000E+12	7.10657E+01	0.99990
N	7.46803E-15	3.84777E-10	5.38870E-09	28	3.0000E+13	6.45805E+00	0.98154
CH	4.41513E-17	2.27482E-12	2.28840E-11	29	3.0000E+13	3.49208E-02	0.99316
HNCO	1.42240E-12	7.32866E-08	-6.26817E-08	30	7.8362E+04	4.99331E-03	1.08001
NCO	1.34495E-14	6.92964E-10	2.97262E-09	31	1.3182E+13	2.54882E+03	1.00000
NH2	3.21244E-13	1.65516E-08	5.63250E-08	32	2.7135E+13	5.24583E+03	0.99986
NO	4.62605E-13	2.38349E-08	1.60872E-07	33	1.0765E+12	5.66568E+02	0.98559
NH	1.58641E-14	8.17373E-10	-2.61956E-09	34	3.0425E+11	1.62444E+02	0.99985
NO2	6.34113E-15	3.26716E-10	-3.17438E-10	35	3.4241E+13	5.62223E+02	0.99925
N2O	6.29665E-13	3.26424E-08	1.55942E-07	36	2.0000E+13	1.69326E+00	0.98159
NHNO2	1.44678E-17	7.45429E-13	-8.41252E-12	37	7.7680E+11	4.05041E+03	1.00000
NHNO3	3.28768E-20	1.69392E-15	6.30472E-15	38	1.2020E+12	1.19115E+01	1.00000
NH2O	4.46481E-17	2.30041E-12	2.28086E-11	39	1.0000E+13	2.73693E+02	1.00000
				40	5.0000E+13	2.73128E+02	0.99654
				41	3.0000E+13	1.30608E+01	1.00000
				42	6.0362E+12	2.62413E+00	0.99856
				43	1.0000E+13	7.16104E+00	1.00000
				44	2.8000E+13	1.71727E+02	0.96201
				45	3.5173E+12	-1.70451E+01	0.43186
				46	4.7567E+12	-8.54546E-01	0.12334
				47	9.9567E+12	-6.80129E+01	0.84251
				48	6.6378E+12	1.57825E+00	0.10300
				49	2.0000E+13	4.61667E+01	1.00000
				50	5.2959E+09	2.32358E+01	0.62293
				51	5.0000E+13	1.56146E+00	1.00000
				52	1.6370E+12	1.83826E+04	0.99999
				53	2.0000E+13	2.36109E+02	1.00000
				54	6.6054E+07	2.29953E+02	0.99871
				55	2.2160E+13	6.99178E+04	0.99998
				56	9.1319E+12	5.77015E+03	0.99993
				57	1.4431E+13	1.64862E+04	0.99999
				58	9.8203E+10	2.25505E+03	0.99967
				59	1.3395E+13	8.90699E+02	0.99993
				60	2.0000E+13	4.93423E+04	0.99958
				61	1.7742E+06	9.99327E+00	0.66944
				62	6.6827E+10	9.99656E+01	0.98073
				63	5.0739E+10	1.39529E+02	0.99728

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TABLE D.2.—Continued.
(o) Concluded.

64	6.6827E+10	5.06215E+02	0.99466
65	3.7000E+12	6.76047E-02	0.99995
66	1.0000E+13	1.41631E+02	1.00000
67	3.8536E+12	1.22159E+04	1.00000
68	6.0625E+10	3.64215E-01	0.99718
69	5.0357E+12	8.33265E+01	0.99447
70	1.8626E+13	6.08322E+01	0.98004
71	5.0000E+12	1.32537E+00	0.99997
72	4.0000E+13	1.05872E+01	1.00000
73	3.0000E+13	5.21839E+04	0.99963
74	3.0000E+13	9.92130E+01	1.00000
75	3.0000E+13	2.74011E+02	1.00000
76	2.0000E+13	3.65857E+01	0.99998
77	5.6970E+12	5.74726E+04	0.99974
78	8.5266E+14	7.09507E+01	0.99998
79	1.4800E+07	3.33836E+01	0.99992
80	3.2398E+11	3.82846E+03	0.99801
81	1.7625E+11	6.76362E+02	1.00000
82	6.5974E+11	4.70486E+03	0.49038
83	3.0111E+12	1.15308E+05	0.95944
84	1.3062E+13	1.19028E+04	0.85874
85	4.2568E+13	2.77096E+03	0.95872
86	3.8846E+13	4.74054E+03	0.99417
87	8.0000E+12	2.68107E+03	0.98856
88	1.0229E+14	6.94330E+03	0.99976
89	1.4379E+11	1.34325E+02	0.98351
90	4.2518E+12	-1.66421E+01	0.94051
91	1.8000E+12	1.97632E+02	0.99932
92	7.8000E+11	3.85206E-02	0.99602
93	1.4779E+12	3.47138E+02	0.75391
94	1.0170E+13	2.15446E+04	0.72280
95	1.8792E+15	-1.18888E+03	0.29180
96	3.8787E+03	-2.22968E+01	0.98384
97	3.5612E+15	5.19979E+00	0.99177
98	6.5929E+03	-8.31950E-01	0.94171
99	1.0434E+02	-9.02043E-02	0.79701
100	8.2652E+08	5.05851E-02	1.00000
101	1.5746E+15	-1.64104E-05	0.12395
102	3.4663E+11	1.43426E-04	0.87625
103	1.2730E+11	-2.53547E-03	0.90738
104	1.2000E+13	1.14214E-05	0.99990
105	5.4983E+13	-8.33520E-04	0.85221
106	1.0314E+13	-1.90100E-02	0.45097
107	1.1702E+13	1.90909E-01	0.96180
108	2.4862E+13	9.03448E-03	0.72554
109	3.7000E+12	-8.13011E-03	0.99971
110	2.0000E+13	5.79929E-03	1.00000
111	1.0000E+13	5.39816E-09	0.99817
112	2.0000E+13	3.20608E-03	0.99945
113	1.3017E+12	2.54700E-06	0.99951
114	2.0000E+12	3.91488E-06	0.99991
115	1.3476E+13	1.20849E-02	0.94934
116	2.3574E+12	1.97377E-02	0.93788
117	8.6033E+12	1.06576E-03	0.90613
118	7.0317E+15	-1.69459E-03	0.53754
119	2.3944E+14	1.80375E-02	0.99619
120	7.8362E+08	-2.13842E-02	0.99980
121	2.0108E+08	-2.68944E-01	0.99999
122	7.8865E+05	2.45908E-01	1.00000
123	4.0000E+12	6.42033E-10	1.00000
124	2.0225E+08	-5.28373E-01	0.97760
125	8.4820E+10	-9.28385E-03	0.88966
126	8.4363E+10	1.13167E-03	1.00000
127	1.6788E+12	7.97228E-03	0.63240
128	1.5896E+10	1.57207E-05	0.93485
129	7.8284E+15	2.13693E-08	0.00039
130	8.6008E+15	1.27928E-05	0.00278
131	5.6000E+12	2.45321E-06	0.92148
132	6.2830E+15	1.73385E-04	0.25773
133	3.6000E+13	9.36237E-05	0.97823

DERIVATIVES (CGS UNITS): T 2.54030E+02 RHO 4.61298E-05 V -9.94097E+03
MIXTURE MOLECULAR WEIGHT 27.98600 TOTAL ENERGY EXCHANGE RATE -1.25658E+10 MASS FRACTION SUM 1.00000000
(CAL-CM#3/G#2/SEC)

COMPUTER TIME (CPU) REQUIRED, FOR THIS STEP - 5.866669E+00 S UP TO THIS TIME - 1.396667E+01 S

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS - 279
TOTAL NO. OF DERIVATIVE EVALUATIONS - 359
TOTAL NO. OF JACOBIAN EVALUATIONS - 18
TOTAL CPU TIME - 13.96667 S

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 16.533325 S

(LSENS) READ DATA FOR NEXT CASE

(p) Case 16

CC 1234567890123456789012345678901234567890123456789012345678901234567890

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LENS METHANE - AIR WITH TAB. AREA PROFILE OF CASE 15, BUT PRINT ASSIG; CASE 16
REPEAT
DISTANCE AREA
  &prob xtb= 0.0,5.0,10.0,15.0,20.0,25.0,30.0,32.0,34.0,36.0,38.0,40.0,42.0,44.0,
  atb= 1200.0,1180.0,1160.0,1140.0,1120.0,1100.0,1080.0,1060.0,1040.0,1020.0,
  1000.0,980.0,960.0,940.0,
  print = 5.0, 12.4954, 22.4363, 43.0002, &end
  &start t=1600.0, mach=2.0, p=1.730, &end
CH4 0.049768
CO2 0.199072
N2 0.75116
CH 0.0000001
END
&solver emax=1.0E-5, atolsp=1.0E-14, &end
FINIS

```

INITIAL CONDITIONS

TIME 0.00000E+00 SEC AREA 1.20000E+03 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE (ATM)	1.73000
VELOCITY (CM/SEC)	155259.65
DENSITY (G/CM*3)	3.71736E-04
TEMPERATURE (DEG K)	1600.00
MASS FLOW RATE (G/SEC)	6.92587E+04
ENTROPY (CAL/G/DEG K)	2.1223
MACH NUMBER	2.0000
GAMMA	1.2780
ENTHALPY (CAL/G)	3.46688E+02
SP. HEAT (CP) (CAL/G/DEG K)	3.23820E-01

INTEGRATION INDICATORS

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STEPS FROM LAST PRINT          0
AVERAGE STEP SIZE              0.00000E+00
METHOD ORDER                    0

TOTAL NUMBER OF STEPS          0
FUNCT EVALUATIONS              0
JACOBIAN EVALUATIONS           0

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CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOL FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION (CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POST- TIVE DIR RATE
CH4	6.55792E-07	4.97680E-02	-4.71274E-06	1	1.9089E+05	1.19373E+01	1.0000E+00
CH3	0.00000E+00	0.00000E+00	4.71274E-06	2	2.9847E+12	0.00000E+00	0.0000E+00
H	0.00000E+00	0.00000E+00	1.64958E-06	3	1.7806E+06	2.21667E+01	1.0000E+00
H2	0.00000E+00	0.00000E+00	0.00000E+00	4	4.7630E+12	0.00000E+00	0.0000E+00
O2	2.62317E-06	1.99072E-01	-8.38235E-05	5	5.1714E+12	0.00000E+00	0.0000E+00
H2O	0.00000E+00	0.00000E+00	3.06316E-06	6	2.9021E+09	0.00000E+00	0.0000E+00
O	0.00000E+00	0.00000E+00	8.07603E-05	7	6.3000E+12	0.00000E+00	0.0000E+00
OH	0.00000E+00	0.00000E+00	0.00000E+00	8	6.7687E+10	0.00000E+00	0.0000E+00
H2O	0.00000E+00	0.00000E+00	0.00000E+00	9	1.2548E+13	0.00000E+00	0.0000E+00
CH3O	0.00000E+00	0.00000E+00	0.00000E+00	10	6.2462E+12	0.00000E+00	0.0000E+00
CH2O	0.00000E+00	0.00000E+00	0.00000E+00	11	9.5679E+12	0.00000E+00	0.0000E+00
C2H6	0.00000E+00	0.00000E+00	0.00000E+00	12	2.8755E+13	0.00000E+00	0.0000E+00
C2H5	0.00000E+00	0.00000E+00	0.00000E+00	13	5.8291E+12	0.00000E+00	0.0000E+00
C2H4	0.00000E+00	0.00000E+00	0.00000E+00	14	4.1501E+11	0.00000E+00	0.0000E+00
CH2	0.00000E+00	0.00000E+00	0.00000E+00	15	4.8000E+13	0.00000E+00	0.0000E+00
C2H3	0.00000E+00	0.00000E+00	0.00000E+00	16	2.0000E+13	0.00000E+00	0.0000E+00
C2H2	0.00000E+00	0.00000E+00	0.00000E+00	17	6.0651E+12	0.00000E+00	0.0000E+00
HCO	0.00000E+00	0.00000E+00	0.00000E+00	18	3.8291E+06	0.00000E+00	0.0000E+00
C2H2O	0.00000E+00	0.00000E+00	0.00000E+00	19	3.2601E+12	0.00000E+00	0.0000E+00
C2H	0.00000E+00	0.00000E+00	0.00000E+00	20	17.4788E+12	0.00000E+00	0.0000E+00
CO	0.00000E+00	0.00000E+00	0.00000E+00	21	2.3129E+12	0.00000E+00	0.0000E+00
C2HO	0.00000E+00	0.00000E+00	0.00000E+00	22	5.1877E+12	0.00000E+00	0.0000E+00
CH	0.00000E+00	0.00000E+00	0.00000E+00	23	1.2768E+11	0.00000E+00	0.0000E+00
CO2	0.00000E+00	0.00000E+00	0.00000E+00	24	4.3056E+12	0.00000E+00	0.0000E+00
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	25	6.0000E+12	0.00000E+00	0.0000E+00
H2	9.89802E-06	7.51160E-01	-1.79633E-12	26	3.3000E+13	0.00000E+00	0.0000E+00
HCH	0.00000E+00	0.00000E+00	0.00000E+00	27	5.0000E+12	0.00000E+00	0.0000E+00
H	0.00000E+00	0.00000E+00	0.00000E+00	28	3.0000E+13	0.00000E+00	0.0000E+00
CN	1.31770E-12	1.00000E-07	-8.07603E-05	29	3.0000E+13	0.00000E+00	0.0000E+00
HNCO	0.00000E+00	0.00000E+00	0.00000E+00	30	1.0180E+02	0.00000E+00	0.0000E+00
HCO	0.00000E+00	0.00000E+00	8.07603E-05	31	7.1320E+12	0.00000E+00	0.0000E+00
NH2	0.00000E+00	0.00000E+00	0.00000E+00	32	1.3995E+13	0.00000E+00	0.0000E+00
HO	0.00000E+00	0.00000E+00	0.00000E+00	33	6.9697E+11	0.00000E+00	0.0000E+00
NH	0.00000E+00	0.00000E+00	0.00000E+00	34	3.0649E+11	0.00000E+00	0.0000E+00
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	35	3.1195E+13	0.00000E+00	0.0000E+00
H2O	0.00000E+00	0.00000E+00	1.79633E-12	36			

TABLE D.2.—Continued.
(p) Continued.

51	3.0000E+13	0.00000E+00	0.00000
52	1.0486E+12	0.00000E+00	0.00000
53	2.0000E+13	0.00000E+00	0.00000
54	4.3141E+05	0.00000E+00	0.00000
55	2.0569E+13	0.00000E+00	0.00000
56	7.1274E+12	0.00000E+00	0.00000
57	1.1604E+13	0.00000E+00	0.00000
58	6.0604E+10	0.00000E+00	0.00000
59	1.2000E+13	0.00000E+00	0.00000
60	2.0000E+13	0.00000E+00	0.00000
61	5.9987E+03	0.00000E+00	0.00000
62	1.1686E+10	0.00000E+00	0.00000
63	8.8532E+09	0.00000E+00	0.00000
64	1.1683E+10	0.00000E+00	0.00000
65	3.7000E+12	0.00000E+00	0.00000
66	1.0000E+13	0.00000E+00	0.00000
67	2.2405E+12	0.00000E+00	0.00000
68	0.066E+10	0.00000E+00	0.00000
69	3.1270E+12	0.00000E+00	0.00000
70	1.726E+13	0.00000E+00	0.00000
71	5.0000E+12	0.00000E+00	0.00000
72	4.0000E+13	0.00000E+00	0.00000
73	1.0000E+13	0.00000E+00	0.00000
74	1.0000E+13	0.00000E+00	0.00000
75	1.0000E+13	0.00000E+00	0.00000
76	2.0000E+13	0.00000E+00	0.00000
77	2.1659E+12	0.00000E+00	0.00000
78	6.6096E+14	0.00000E+00	0.00000
79	2.6523E+05	0.00000E+00	0.00000
80	3.0447E+11	0.00000E+00	0.00000
81	4.2421E+10	0.00000E+00	0.00000
82	2.1085E+11	0.00000E+00	0.00000
83	0.872E+12	0.00000E+00	0.00000
84	5.5602E+12	0.00000E+00	0.00000
85	3.7302E+13	0.00000E+00	0.00000
86	3.6507E+13	0.00000E+00	0.00000
87	8.0000E+12	0.00000E+00	0.00000
88	9.5708E+13	0.00000E+00	0.00000
89	3.0432E+10	0.00000E+00	0.00000
90	3.8905E+12	0.00000E+00	0.00000
91	3.8000E+12	0.00000E+00	0.00000
92	7.8000E+11	0.00000E+00	0.00000
93	8.7496E+10	0.00000E+00	0.00000
94	6.9635E+12	0.00000E+00	0.00000
95	1.9996E+15	0.00000E+00	0.00000
96	5.6558E+00	0.00000E+00	0.00000
97	4.4375E+15	0.00000E+00	0.00000
98	6.960E+01	0.00000E+00	0.00000
99	8.5187E-02	2.15082E-05	1.00000
100	2.5393E+08	0.00000E+00	0.00000
101	1.1329E+13	0.00000E+00	0.00000
102	0.0387E+11	0.00000E+00	0.00000
103	1.6581E+11	0.00000E+00	0.00000
104	2.000E+13	0.00000E+00	0.00000
105	7.877E+13	0.00000E+00	0.00000
106	8.974E+12	0.00000E+00	0.00000
107	6.9017E+12	0.00000E+00	0.00000
108	2.3364E+13	5.84425E+02	1.00000
109	2.7000E+12	0.00000E+00	0.00000
110	2.0000E+13	0.00000E+00	0.00000
111	1.0000E+13	0.00000E+00	0.00000
112	2.0000E+13	0.00000E+00	0.00000
113	2.0207E+11	0.00000E+00	0.00000
114	2.0000E+12	0.00000E+00	0.00000
115	1.0662E+13	0.00000E+00	0.00000
116	2.4283E+12	0.00000E+00	0.00000
117	8.2907E+12	0.00000E+00	0.00000
118	8.0944E+15	0.00000E+00	0.00000
119	2.1854E+14	0.00000E+00	0.00000
120	2.4219E+07	0.00000E+00	0.00000
121	1.3584E+07	0.00000E+00	0.00000
122	6.9185E+03	0.00000E+00	0.00000
123	6.0000E+12	0.00000E+00	0.00000
124	8.9376E+06	0.00000E+00	0.00000
125	1.4882E+10	-1.29992E-05	1.00000
126	1.5945E+10	0.00000E+00	0.00000
127	6.5717E+11	0.00000E+00	0.00000
128	6.6242E+09	0.00000E+00	0.00000
129	6.9124E+15	0.00000E+00	0.00000
130	6.5587E+15	0.00000E+00	0.00000
131	5.0000E+12	0.00000E+00	0.00000
132	6.5215E+15	0.00000E+00	0.00000
133	2.6000E+13	0.00000E+00	0.00000
DERIVATIVES (CGS UNITS): T			
1.97928E+00 RHO			
1.65526E-06 V			
-1.72834E+02			
MIXTURE MOLECULAR WEIGHT			
28.21102			
TOTAL ENERGY EXCHANGE RATE			
-1.27744E+06			
MASS FRACTION SUM			
1.00000000			
CPU TIME FOR INITIALIZATION OF LSENS =			
1.659992 S			

TABLE D.2.—Continued.
(p) Continued.

TIME	1.46451E-04	SEC	AREA	1.10936E+03	SQ CM	AXIAL POSITION	2.24363E+01	CM
FLOW PROPERTIES					INTEGRATION INDICATORS			
PRESSURE (ATM)	1.98504		STEPS FROM LAST PRINT		29			
VELOCITY (CM/SEC)	150959.76		AVERAGE STEP SIZE		0.35712E+00			
DENSITY (G/CM**3)	4.13563E-04		METHOD ORDER		4			
TEMPERATURE (DEG K)	1650.17		TOTAL NUMBER OF STEPS		161			
MASS FLOW RATE (G/SEC)	6.92587E+04		FUNCT EVALUATIONS		199			
ENTROPY (CAL/G/DEG K)	2.1234		JACOBIAN EVALUATIONS		25			
MACH NUMBER	1.9161							
GAMMA	1.2763							
ENTHALPY (CAL/G)	3.62423E+02							
SP. HEAT (CP) (CAL/G/DEG K)	3.25371E-01							
CHEMICAL PROPERTIES								
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE	
CH4	7.17624E-07	4.89515E-02	-2.51430E-04	1	4.4284E+05	2.65382E+01	0.97428	0.97428
CH3	3.70822E-09	2.52950E-04	5.03006E-05	2	3.3445E+12	9.58538E+01	0.97496	0.97496
H	7.00622E-12	4.77918E-07	1.25105E-07	3	3.0419E+06	2.82779E+01	0.76098	0.76098
H2	7.91113E-10	5.39645E-05	1.66017E-05	4	5.3278E+12	3.79712E+02	0.99957	0.99957
O2	2.91153E-06	1.98605E-01	-1.46771E-04	5	5.4252E+12	9.45847E+02	0.99824	0.99824
H2O	9.44564E-10	6.44319E-05	7.30120E-06	6	3.8178E+09	2.40782E+02	0.99910	0.99910
O	1.69934E-11	1.15918E-06	2.71685E-07	7	6.3000E+12	-9.40211E+00	0.62316	0.62316
OH	4.16255E-11	2.83942E-06	7.69568E-07	8	8.2740E+10	1.72728E+02	1.00000	1.00000
H2O	7.12085E-09	4.85737E-04	1.68311E-04	9	1.2394E+13	2.67192E+02	0.26815	0.26815
CH3O	2.43557E-11	1.66139E-06	4.42876E-07	10	6.8533E+12	5.08339E-01	1.00000	1.00000
CH2O	4.35616E-09	2.97149E-04	1.03105E-04	11	1.0314E+13	1.85554E+00	1.00000	1.00000
C2H6	1.81074E-09	1.23516E-04	4.30530E-05	12	2.9739E+13	1.31057E+01	1.00000	1.00000
C2H5	2.28401E-14	1.55800E-09	7.69218E-10	13	7.8404E+12	1.53007E+01	0.99685	0.99685
C2H4	5.74155E-11	3.91650E-06	2.72325E-06	14	4.3534E+11	1.64308E-01	0.97073	0.97073
CH2	1.33148E-15	9.08248E-11	6.47923E-11	15	4.8000E+13	4.47720E-05	0.99693	0.99693
C2H3	6.99640E-16	4.77249E-11	4.59943E-11	16	2.0000E+13	5.77223E-04	0.99976	0.99976
C2H2	1.40319E-13	9.57163E-09	8.59544E-09	17	6.6865E+12	1.57259E-02	0.99998	0.99998
HCO	4.83643E-14	3.29909E-09	1.94312E-09	18	8.1738E+06	4.02253E-02	1.00000	1.00000
C2H2O	3.63528E-16	2.47974E-11	2.56030E-11	19	3.2987E+12	4.60940E-02	1.00000	1.00000
C2H	4.71927E-20	3.21917E-15	3.59995E-15	20	1.4924E+12	-6.02946E-01	0.96657	0.96657
CO	1.30390E-10	8.89437E-06	6.00064E-06	21	2.3381E+12	1.33377E-02	1.00000	1.00000
C2HO	2.00636E-17	1.36861E-12	1.57302E-12	22	5.4417E+12	3.10424E-02	0.99998	0.99998
CH	1.04070E-20	7.09899E-16	7.22929E-16	23	1.7339E+11	1.03905E-02	0.99930	0.99930
CO2	1.42215E-13	9.70086E-09	8.80830E-09	24	4.2953E+12	5.11572E-02	1.00000	1.00000
H2O2	8.54763E-13	5.83063E-08	1.03216E-08	25	6.0000E+12	1.71843E-07	0.99932	0.99932
H2	1.10117E-05	7.51146E-01	-9.52715E-11	26	3.3000E+13	2.29396E-06	1.00000	1.00000
HCN	4.10904E-18	2.80291E-13	1.90069E-13	27	5.0000E+12	8.51337E-07	0.99995	0.99995
N	1.46100E-18	9.96595E-14	4.38094E-14	28	3.0000E+13	-3.29912E-09	0.95281	0.95281
CN	5.12271E-18	3.49438E-13	1.22003E-13	29	3.0000E+13	4.32689E-15	0.74712	0.74712
HNCO	2.59465E-13	1.76990E-08	5.95719E-09	30	2.8320E+02	3.39666E-09	0.99724	0.99724
NCO	1.17461E-12	8.01242E-08	-6.53491E-09	31	7.8394E+12	1.09293E-04	1.00000	1.00000
NH2	2.97443E-16	2.02896E-11	1.36082E-11	32	1.5497E+13	2.16050E-04	1.00000	1.00000
NO	2.14401E-14	1.46250E-09	3.66047E-10	33	7.4517E+11	2.54429E-05	0.99981	0.99981
NH	8.96606E-15	6.11606E-10	1.60472E-10	34	3.0107E+11	1.02814E-05	0.99999	0.99999
NO2	1.38841E-15	9.47084E-11	4.26104E-11	35	3.1645E+13	2.54227E-05	1.00000	1.00000
N2O	4.48392E-15	3.05864E-10	9.25858E-11	36	2.0000E+13	2.29332E-10	0.99835	0.99835
HNH2	1.76861E-20	1.20643E-15	-5.84729E-16	37	6.8116E+11	2.32647E-04	1.00000	1.00000
HNH3	1.71978E-22	1.17312E-17	7.01639E-18	38	1.2020E+12	2.39613E-09	1.00000	1.00000
HHO	6.02738E-20	4.11148E-15	1.98167E-15	39	1.0000E+13	4.88249E-08	0.99990	0.99990
				40	5.0000E+13	3.98352E-08	0.96936	0.96936
				41	3.0000E+13	4.68576E-12	0.99999	0.99999
				42	5.4340E+12	-2.84658E-12	0.77032	0.77032
				43	1.0000E+13	2.35361E-14	1.00000	1.00000
				44	2.8000E+13	-1.17593E-04	0.97937	0.97937
				45	3.0043E+12	2.56633E-07	0.96552	0.96552
				46	3.9726E+12	-2.76520E-05	0.99787	0.99787
				47	6.5394E+12	4.95945E-08	0.50928	0.50928
				48	4.3596E+12	1.56134E-07	0.99156	0.99156
				49	2.0000E+13	7.22376E-07	1.00000	1.00000
				50	2.2625E+08	6.94083E-06	0.98456	0.98456
				51	5.0000E+13	2.34445E-10	1.00000	1.00000
				52	1.1231E+12	4.65628E+02	1.00000	1.00000
				53	2.0000E+13	1.99541E-02	1.00000	1.00000
				54	9.3599E+05	3.49479E-01	1.00000	1.00000
				55	2.0806E+13	2.20584E+01	1.00000	1.00000
				56	7.4046E+12	1.32131E+00	1.00000	1.00000
				57	1.2001E+13	5.19400E+00	1.00000	1.00000
				58	6.5181E+10	6.15586E+00	0.99996	0.99996
				59	1.2187E+13	1.27778E-02	0.99991	0.99991
				60	2.0000E+13	4.09585E+02	1.00000	1.00000
				61	1.4403E+04	4.57785E-03	0.99997	0.99997
				62	1.5254E+10	2.31704E-03	0.99997	0.99997
				63	1.1560E+10	4.25901E-03	1.00000	1.00000
				64	1.5254E+10	1.37665E-02	1.00000	1.00000
				65	3.7000E+12	-5.25067E-15	0.14089	0.14089
				66	1.0000E+13	1.77160E-06	1.00000	1.00000
				67	2.4319E+12	5.51212E-02	1.00000	1.00000
				68	1.3688E+10	1.81075E-09	1.00000	1.00000
				69	3.3600E+12	1.08878E-06	0.99998	0.99998
				70	1.2566E+13	6.85208E-07	0.99976	0.99976
				71	5.0000E+12	5.18177E-11	0.99982	0.99982
				72	4.0000E+13	4.14617E-10	1.00000	1.00000
				73	3.0000E+13	2.46987E+01	0.99998	0.99998
				74	3.0000E+13	1.44159E-04	1.00000	1.00000
				75	1.0000E+13	3.53120E-04	1.00000	1.00000
				76	2.0000E+13	3.96237E-05	1.00000	1.00000
				77	2.5136E+12	1.04200E+01	1.00000	1.00000
				78	6.8739E+14	1.30550E-04	1.00000	1.00000
				79	1.2074E+06	2.67994E-03	1.00000	1.00000
				80	3.0739E+11	9.75453E-03	0.99997	0.99997
				81	5.2820E+10	3.80361E-02	1.00000	1.00000

TABLE D.2.—Continued.
(p) Continued.

82	2.5132E+11	1.34282E-01	0.75519
83	1.2718E+12	1.51638E-02	0.99966
84	6.3415E+12	4.89878E-01	0.98280
85	3.8068E+13	1.31865E+00	0.89525
86	3.6858E+13	3.45282E+00	0.99820
87	8.0000E+12	1.82553E+00	0.99264
88	9.6693E+13	3.74133E+00	1.00000
89	3.8651E+10	1.67619E-01	0.99261
90	3.9440E+12	-6.97879E-03	0.89480
91	1.8000E+12	9.38246E+00	0.99923
92	7.8000E+11	2.73111E-05	0.99999
93	1.3520E+11	9.49668E+00	0.99992
94	7.3817E+12	1.32157E+00	0.92973
95	7.9806E+15	-5.71788E-01	0.89258
96	1.5457E+01	-1.90679E-04	0.91359
97	4.3026E+15	4.31723E-05	0.98325
98	4.2473E+01	-1.53312E-07	0.02648
99	2.5532E-01	6.24295E-05	0.97979
100	3.0453E+08	2.04045E-10	1.00000
101	1.1918E+13	2.82378E-07	0.99991
102	1.2468E+11	-9.51699E-09	0.99668
103	1.7030E+11	-8.19196E-07	0.99979
104	1.2000E+13	6.10771E-09	1.00000
105	4.0114E+13	-7.76301E-05	0.99936
106	6.4274E+12	3.49108E-02	0.99972
107	7.4861E+12	7.95645E-05	0.99997
108	2.3589E+13	9.75762E-04	0.47435
109	3.7000E+12	8.99143E-04	1.00000
110	2.0000E+13	2.33411E-03	1.00000
111	1.0000E+13	1.00337E-10	1.00000
112	2.0000E+13	9.62332E-04	1.00000
113	7.7207E+11	9.97604E-16	0.99044
114	2.0000E+12	2.40178E-15	0.99717
115	1.1037E+13	2.40839E-05	0.99999
116	2.4172E+12	2.85250E-04	0.99662
117	8.3381E+12	5.36940E-07	0.46681
118	8.0051E+15	-2.29534E-05	0.98923
119	2.2164E+14	1.26033E-05	0.99982
120	5.5414E+07	1.46332E-08	0.99669
121	2.0808E+07	-3.95127E-05	1.00000
122	1.4344E+04	1.56954E-05	1.00000
123	4.0000E+12	4.74400E-14	1.00000
124	1.5404E+07	-5.04530E-04	0.98840
125	1.9454E+10	-3.69577E-05	0.99977
126	2.0569E+10	9.16356E-09	1.00000
127	7.5925E+11	-6.18438E-08	0.30722
128	3.4628E+09	2.22362E-08	0.99981
129	9.5586E+15	4.10234E-11	0.00092
130	9.4045E+15	-1.88154E-08	0.02549
131	5.0000E+12	1.70434E-12	0.12131
132	6.4842E+15	1.20709E-08	0.14458
133	3.6000E+13	4.85856E-10	0.92002

DERIVATIVES (CGS UNITS): T 2.88791E+00 RHO 2.20037E-06 V -2.27804E+02
MIXTURE MOLECULAR HEIGHT 28.21051 TOTAL ENERGY EXCHANGE RATE -4.25919E+07 MASS FRACTION SUM 1.00000000
(CAL-CM**3/G**2/SEC)

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 1.660004E+00 S UP TO THIS TIME - 9.010025E+00 S

TIME	2.83463E-04	SEC	AREA	9.54999E+02	SQ CM	AXIAL POSITION	4.25001E+01	CM
FLOW PROPERTIES			INTEGRATION INDICATORS					
PRESSURE (ATM)	3.17520		STEPS FROM LAST PRINT	118				
VELOCITY (CM/SEC)	133515.39		AVERAGE STEP SIZE	0.16567E+00				
DENSITY (G/CM**3)	5.43171E-04		METHOD ORDER	4				
TEMPERATURE (DEG K)	1993.73							
MASS FLOW RATE (G/SEC)	6.92581E+04		TOTAL NUMBER OF STEPS	279				
ENTROPY (CAL/G/DEG K)	2.1774		FUNCT EVALUATIONS	359				
MACH NUMBER	1.5379		JACOBIAN EVALUATIONS	38				
GAMMA	1.2725							
ENTHALPY (CAL/G)	4.21726E+02							
SP. HEAT (CP) (CAL/G/DEG K)	3.31576E-01							
CHEMICAL PROPERTIES								
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DER	RATE
CH4	3.40620E-07	1.75499E-02	-6.38715E-02	1	5.5143E+07	-2.98280E+03	0.74676	
CH3	1.27895E-07	6.58958E-03	1.67178E-02	2	5.2504E+12	1.95436E+04	0.76983	
H2	3.51808E-09	1.81263E-04	1.43144E-03	3	5.7700E+07	-1.02023E+03	0.82066	
H2	4.92203E-08	2.53600E-03	3.55768E-03	4	7.8633E+12	7.00692E+04	0.96749	
O2	3.34689E-06	1.72443E-01	-6.64127E-02	5	7.0591E+12	1.34024E+05	0.93620	
HO2	5.6934E-09	2.93344E-04	2.42879E-04	6	1.7232E+10	2.31964E+04	0.92779	
O	6.36007E-09	3.27693E-04	2.81061E-03	7	6.3000E+12	-3.74580E+04	0.43833	
OH	1.75657E-08	9.05044E-04	7.32672E-03	8	2.4945E+11	1.62441E+04	1.00000	
H2O	6.74506E-07	3.47529E-02	8.94564E-02	9	1.1491E+13	6.62581E+04	0.10401	
CH3O	9.89912E-10	5.10037E-05	6.96517E-05	10	1.1410E+13	3.96674E+03	0.99999	
CH2O	5.29894E-08	2.73019E-03	-5.09736E-03	11	1.5580E+13	9.79289E+03	0.99999	
C2H6	2.91577E-08	1.50231E-03	-2.83738E-03	12	3.5782E+13	6.21155E+04	0.99998	
C2H5	3.55715E-11	1.83277E-06	8.32578E-06	13	3.9978E+13	7.56601E+04	0.80876	
C2H4	7.70959E-08	3.97224E-03	7.73785E-03	14	5.6616E+11	1.66765E+02	0.72996	
CH2	2.79405E-10	1.43959E-05	1.57649E-04	15	4.8000E+13	2.01330E+01	0.98885	
C2H3	2.38695E-10	1.22984E-05	1.09986E-04	16	2.0000E+13	2.42113E+03	0.99948	
C2H2	8.96751E-09	4.62037E-04	2.59869E-03	17	1.1428E+13	1.04961E+04	0.99904	

TABLE D.2.—Continued.

(p) Continued.

HCO	1.53382E-10	7.90275E-06	4.93072E-05	18	5.2749E+08	2.67525E+03	0.99999
C2H2O	1.07055E-10	5.51584E-06	5.17669E-05	19	3.5189E+12	1.61480E+04	0.99973
C2H	1.44824E-12	7.46182E-08	1.08673E-06	20	1.5696E+12	6.83826E+03	0.94913
CO	1.98853E-07	1.02456E-02	3.46313E-02	21	2.4811E+12	4.12349E+03	1.00000
C2HO	4.59564E-10	2.36783E-05	3.20663E-04	22	7.0770E+12	1.17600E+04	0.99986
CH	1.24818E-12	6.43104E-08	1.27865E-06	23	9.3180E+11	1.45422E+04	0.99390
CO2	4.31761E-09	2.22458E-04	1.35970E-03	24	4.2392E+12	1.14789E+04	1.00000
H2O2	4.15756E-12	2.14212E-07	4.19630E-07	25	6.0000E+12	1.70715E+01	0.99964
N2	1.44627E-05	7.45169E-01	-2.43711E-07	26	5.3000E+13	1.69803E+02	1.00000
HCH	2.20257E-14	1.13484E-09	1.56221E-08	27	5.0000E+12	7.10497E+01	0.99990
H	7.46662E-15	3.84706E-10	5.38724E-09	28	3.0000E+13	6.65628E+00	0.98154
CH	4.41453E-17	2.27452E-12	2.28789E-11	29	3.0000E+13	3.49100E-02	0.99316
HICO	1.42241E-12	7.32875E-08	-6.26747E-08	30	7.8352E+04	4.99591E-03	0.10809
NCO	1.34487E-14	6.92925E-10	2.97220E-09	31	1.3182E+13	2.54831E+03	1.00000
NH2	3.21229E-13	1.65508E-08	5.63190E-08	32	2.7135E+13	5.24478E+03	0.99986
NO	4.62562E-13	2.38328E-08	1.60839E-07	33	1.0765E+12	5.66461E+02	0.98559
NH	1.58648E-14	8.17408E-10	-2.61949E-09	34	3.0425E+11	1.62415E+02	0.99985
NO2	6.34119E-15	3.26720E-10	-3.17522E-10	35	3.4241E+13	5.62117E+02	0.99925
N2O	6.29623E-13	3.24404E-08	1.55920E-07	36	2.0000E+13	1.69276E+00	0.98159
HNO2	1.44656E-17	7.45318E-13	-8.41042E-12	37	7.7679E+11	4.04949E+03	1.00000
HNO3	3.28750E-20	1.69383E-15	6.30338E-15	38	1.2020E+12	1.19080E+01	1.00000
HNO	4.46421E-17	2.30011E-12	2.28034E-11	39	1.0000E+13	2.73614E+02	1.00000
				40	5.0000E+13	2.73051E+02	0.99654
				41	3.0000E+13	1.30566E+01	1.00000
				42	6.0362E+12	2.62327E+00	0.99856
				43	1.0000E+13	7.15847E+00	1.00000
				44	2.8000E+13	1.71686E+02	0.96201
				45	3.5173E+12	-1.70409E+01	0.43186
				46	4.7567E+12	-8.55105E-01	0.12344
				47	9.9566E+12	-6.79987E+01	0.84252
				48	6.6377E+12	1.57859E+00	0.10305
				49	2.0000E+13	4.61558E+01	1.00000
				50	5.2955E+09	2.32313E+01	0.62292
				51	5.0000E+13	1.56099E+00	1.00000
				52	1.6369E+12	1.83822E+04	0.99999
				53	2.0000E+13	2.36080E+02	1.00000
				54	6.6048E+07	2.29938E+02	0.99871
				55	2.2160E+13	6.99119E+04	0.99998
				56	9.1319E+12	5.76966E+03	0.99993
				57	1.4431E+13	1.64847E+04	0.99999
				58	9.8202E+10	2.25501E+03	0.99967
				59	1.3395E+13	8.90594E+02	0.99993
				60	2.0000E+13	4.93401E+04	0.99958
				61	1.7740E+06	9.99241E+00	0.66947
				62	6.6825E+10	9.99487E+01	0.98073
				63	5.0737E+10	1.39504E+02	0.99728
				64	6.6825E+10	5.06128E+02	0.99666
				65	3.7000E+12	6.75815E-02	0.99995
				66	1.0000E+13	1.41594E+02	1.00000
				67	3.8535E+12	1.22140E+04	1.00000
				68	6.0623E+10	3.64109E-01	0.99718
				69	5.0356E+12	8.33047E+01	0.99447
				70	1.8626E+13	6.08166E+01	0.98004
				71	5.0000E+12	1.32298E+00	0.99997
				72	4.0000E+13	1.05841E+01	1.00000
				73	3.0000E+13	5.21798E+04	0.99963
				74	3.0000E+13	9.91935E+01	1.00000
				75	3.0000E+13	2.73959E+02	1.00000
				76	2.0000E+13	3.65788E+01	0.99998
				77	5.6969E+12	5.74668E+04	0.99974
				78	8.5266E+14	7.09389E+01	0.99998
				79	1.4799E+07	3.33805E+01	0.99992
				80	3.2398E+11	3.82805E+03	0.99801
				81	1.7624E+11	6.76307E+02	1.00000
				82	6.5972E+11	4.70431E+03	0.49041
				83	3.0110E+12	1.15295E+05	0.95944
				84	1.3061E+13	1.19012E+04	0.85875
				85	4.2568E+13	2.77063E+03	0.95872
				86	3.8846E+13	4.73994E+03	0.99417
				87	8.0000E+12	2.68075E+03	0.98856
				88	1.0229E+14	6.94249E+03	0.99976
				89	1.4378E+11	1.34318E+02	0.98351
				90	4.2518E+12	-1.66407E+01	0.94052
				91	1.8000E+12	1.97628E+02	0.99932
				92	7.8000E+11	3.85156E-02	0.99602
				93	1.4778E+12	3.47126E+02	0.75394
				94	1.0170E+13	2.15420E+04	0.72281
				95	1.8792E+15	-1.18888E+03	0.20182
				96	3.8783E+03	-2.22921E+01	0.98384
				97	3.5612E+15	5.19866E+00	0.99177
				98	6.5922E+03	-8.31771E-01	0.94171
				99	1.0433E+02	-9.01815E-02	0.79699
				100	8.2650E+08	5.05707E-02	1.00000
				101	1.5746E+13	-1.63874E-05	0.12382
				102	3.4462E+11	1.43379E-04	0.87624
				103	1.9730E+11	-2.53524E-03	0.90740
				104	1.2000E+13	1.14186E-05	0.99990
				105	5.4983E+13	-8.33371E-04	0.85222
				106	1.0314E+13	-1.90072E-02	0.45096
				107	1.1701E+13	1.90890E-01	0.96180
				108	2.4862E+13	9.03348E-03	0.72555
				109	3.7000E+12	-8.12931E-03	0.99971
				110	2.0000E+13	5.79830E-03	1.00000

TABLE D.2.—Concluded.
(p) Concluded.

111	1.0000E+13	3.39733E-09	0.99817
112	2.0000E+13	3.20557E-03	0.99945
113	1.3017E+12	2.54607E-06	0.99951
114	2.0000E+12	3.91350E-06	0.99991
115	1.3476E+13	1.20841E-02	0.94934
116	2.3574E+12	1.97357E-02	0.93788
117	8.6033E+12	1.06566E-03	0.90613
118	7.5317E+15	-1.69469E-03	0.53760
119	2.3944E+14	1.80359E-02	0.99819
120	7.8357E+08	-2.13779E-02	0.99980
121	2.2107E+08	-2.68891E-01	0.99999
122	7.8859E+05	2.45860E-01	1.00000
123	4.0000E+12	6.41922E-10	1.00000
124	2.9223E+08	-5.28300E-01	0.97760
125	8.4817E+10	-9.28288E-03	0.88967
126	9.3361E+10	1.13144E-03	1.00000
127	1.6788E+12	7.97087E-03	0.63240
128	1.5695E+10	1.57204E-05	0.93487
129	7.8284E+15	2.13649E-08	0.00039
130	3.6008E+15	1.27862E-05	0.00278
131	5.0000E+12	2.45262E-06	0.92147
132	5.2830E+15	1.73344E-04	0.25772
133	3.6000E+13	9.36013E-05	0.97823

DERIVATIVES (CGS UNITS): T 2.54007E+02 RHO 4.61257E-05 V -9.94004E+03
MIXTURE MOLECULAR HEIGHT 27.98601 TOTAL ENERGY EXCHANGE RATE -1.25348E+10 MASS FRACTION SUM 1.00000001
(CAL-CM**3/G**2/SEC)

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 5.866669E+00 S UP TO THIS TIME - 1.390001E+01 S

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS - 279
TOTAL NO. OF DERIVATIVE EVALUATIONS - 359
TOTAL NO. OF JACOBIAN EVALUATIONS - 38
TOTAL CPU TIME - 13.900009 S

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 15.649994 S

(LSENS) READ DATA FOR NEXT CASE

Appendix E

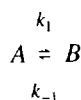
Sensitivity Test Cases

In addition to the kinetics-only test cases described in appendix D we have prepared a set of nine kinetics-plus-sensitivity-analysis test cases. These example problems are also supplied with LSENS. The first six cases are constant-temperature problems whose results have been published in the literature. Results for cases 1 and 2 were also computed analytically. Excellent agreement between the LSENS and literature results was obtained for all cases. The last three cases are non-isothermal problems that illustrate the application of sensitivity analysis to combustion problems. As for the kinetics-only test cases, all sensitivity cases are set up in one file for execution in a single computer run. Cases 1, 2, 5, and 7 involve dummy species used in simple reactions. The thermodynamic data for these species are not read from the standard thermodynamic data file. Their coefficients are placed at the beginning of the problem data file. In this appendix we describe these cases. We then list the complete input file in table E.1. Cases 8 and 9 will be especially useful to users as models for their own sensitivity analysis computations.

Description of Test Cases

Case 1

Case 1 is the constant-volume isothermal reaction



where k_1 and k_{-1} , the forward and reverse rate coefficients, are given separately by writing the two separate irreversible reactions $A \rightarrow B$ and $B \rightarrow A$. This case was first studied by Hwang (ref. 12) and was later used by Radhakrishnan (ref. 13) to compare sensitivity analysis methods. Note that in namelist PROB both the variables SENSTD and SENCAL are set equal to TRUE. This action tells LSENS to compute sensitivity coefficients for the time derivatives of the

dependent variables as well as for the variables themselves. The variable ALLSP is used after the keyword INIT to obtain initial value sensitivities with respect to all species and after the keyword SENSVAR to obtain sensitivities for all species concentrations at each print station. In namelist SENRXN we have set ALLRXN equal to TRUE to obtain sensitivities with respect to all reactions. For this and all other isothermal reactions only the variable SENSJ is set equal to TRUE for sensitivities with respect to the preexponential factors. Coefficients with respect to the temperature exponent and activation energy of any reaction will be the same as those for the preexponential factor.

Case 2

Case 2 is the constant-volume isothermal reaction $A \rightleftharpoons B \rightleftharpoons C$. Each forward and reverse reaction is written separately, so that the case has four reactions, $A \rightarrow B$, $B \rightarrow A$, $B \rightarrow C$, and $C \rightarrow B$. This test case was used by Hwang et al. (ref. 14). The keyword INIT does not appear in the sensitivity analysis data, and therefore no sensitivities with respect to initial conditions are computed.

Case 3

Case 3 is the constant-volume isothermal pyrolysis of ethane using the mechanism of Kramer et al. (ref. 15). This same case was also used by Dunker (ref. 16) and Radhakrishnan (refs. 13 and 17) to compare sensitivity analysis methods. The data require sensitivities for all species with respect to the initial ethane concentration and temperature and for all species with respect to the rate coefficients of reactions 1 and 2.

Case 4

Case 4 is the isothermal constant-volume ignition of a methane-oxygen-argon mixture containing trace concentra-

E. Sensitivity Test Cases

tions of carbon dioxide and hydrogen. The mechanism is that of Boni and Penner (ref. 18). Sensitivity coefficients for all species with respect to all reaction preexponential coefficients are required. Separate forward and reverse rate coefficients are given for the reversible reactions.

Case 5

Case 5 is the isothermal, constant-volume oxidation of formaldehyde using the mechanism of Dougherty et al. (ref. 19). In this case the variable TINY is set equal to 0.1 in namelist PROB to set equal to zero any sensitivity coefficients whose magnitudes are less than 0.1. Also, in namelist SENRXN the variable ORDER is set equal to TRUE in order to have a second type of table printed out for the sensitivity coefficients. The second table is organized by dependent variable, and for each one the coefficients are listed in order of decreasing magnitude. The rate-controlling reactions can then be seen at a glance. Note that the chemical mechanism has two reactions that simulate the destruction of species at the wall of the reaction chamber. These are $\text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O}_2\text{W}$ and $\text{HO}_2 \rightarrow \text{HO}_2\text{W}$, where the species on the right side of each reaction has the same thermodynamic properties as the species on the left side.

Case 6

Problem 6 is the isothermal, constant-volume oxidation of wet carbon monoxide. We use the mechanism of Yetter et al. (ref. 20). Sensitivity coefficients with respect to all rate parameters for concentrations of the two variables hydrogen and carbon monoxide are to be computed, as are sensitivities with respect to six initial concentrations. In namelist SENRXN we have set ORDER equal to TRUE and have also set the variable OUTPUT equal to FALSE. This suppresses the printing of the standard type of sensitivity-coefficient table. Only the table organized by dependent variable is printed.

Case 7

Case 7 is the first nonisothermal case, the constant-pressure, irreversible conversion of one reactant to one product with the rate coefficient expression

$$k = 1.0T$$

This test problem, first used by Radhakrishnan (refs. 13 and 17), can be solved analytically and so permits an objective evaluation of the accuracy of the code. Sensitivity coefficients of all dependent variables and their derivatives are required. This is done very simply by placing the one word ALL on the line after the keyword SENSVAR and setting the

variable SENSTD equal to TRUE in namelist PROB. The word ALL is also placed after the keyword INIT to obtain sensitivity coefficients with respect to the initial values of all dependent variables. In namelist SENRXN we have set the variables SENSNJ and SENSEJ as well as SENSJ equal to TRUE in order to obtain sensitivity coefficients with respect to all three rate coefficient parameters in this nonisothermal reaction.

Case 8

Case 8 is the constant-pressure static ignition of a stoichiometric hydrogen-air mixture seeded with 0.45 mol % nitric oxide to catalyze the low-initial-temperature (950.66 K) reaction. The mechanism is the same as that used for kinetics test case 2 and described in appendix D. Four reactions of carbon monoxide and carbon dioxide have also been added because the air contains a small amount of carbon dioxide. The latter reactions and rate coefficients are also taken from the kinetics test cases. The variable TINY is set to 1.0×10^{-7} in namelist PROB. Sensitivity coefficients are required for seven dependent variables, six species concentrations and temperature. Initial value sensitivities are required for eight variables. Note that this list is ended by inserting a blank line because there are exactly eight names written on the line following the keyword INIT. Rate coefficient sensitivities are to be computed for the six reactions whose numbers are listed in the array RXNUM in namelist SENRXN.

Case 9

Problem 9 is the constant-volume static ignition of a stoichiometric benzene-oxygen mixture that has been shock heated to an initial temperature of 1405 K. The chemical mechanism was developed by Bittker (ref. 21) to match a wide range of experimental ignition delay times and composition profile data reported for this fuel. Sensitivity coefficients for 10 dependent variables are required, including temperature, density, and pressure. Sensitivities with respect to the initial values of five variables, including temperature and density, will be computed as well as sensitivities to the rate parameters A_j and E_j for 24 reactions listed in the array RXNUM.

Listing of Results

The test case file in table E.1 was also executed on the Sun SPARCstation 1 that was used to execute the kinetics-only cases. Total execution time for the nine cases was approximately 139 s. Sample results are given in table E.2. Of course, these cases too will execute more rapidly on the newer workstations and mainframe computers.

TABLE E.1.—PROBLEM DATA FILE FOR SENSITIVITY ANALYSIS TEST CASES

```

CARD
300.000 1000.000 5000.000
DUMA L 5/66A 1.00 0.00 0.00 0.0 G 300.000 5000.000 1.0 1
0.25161474E 01 0.00000000 0.00000000 0.00000000 0.00000000 2
0.00000000 0.00000000 0.25161474E 01 0.00000000 0.00000000 3
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 4
DUMB L 5/66A 1.00 0.00 0.00 0.0 G 300.000 5000.000 1.0 1
0.25161474E 01 0.00000000 0.00000000 0.00000000 0.00000000 2
0.00000000 0.00000000 0.25161474E 01 0.00000000 0.00000000 3
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 4
DUMC L 5/66A 1.00 0.00 0.00 0.0 G 300.000 5000.000 1.0 1
0.25161474E 01 0.00000000 0.00000000 0.00000000 0.00000000 2
0.00000000 0.00000000 0.25161474E 01 0.00000000 0.00000000 3
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 4
DUMP L 5/66A 1.00 0.00 0.00 0.0 G 300.000 5000.000 1.0 1
0.25161474E 01 0.00000000 0.00000000 0.00000000 0.00000000 2
-0.25161474E 04 0.00000000 0.25161474E 01 0.00000000 0.00000000 3
0.00000000 0.00000000 -0.25161474E 04 0.00000000 0.00000000 4
DUMR L 5/66A 1.00 0.00 0.00 0.0 G 300.000 5000.000 1.0 1
0.25161474E 01 0.00000000 0.00000000 0.00000000 0.00000000 2
0.00000000 0.00000000 0.25161474E 01 0.00000000 0.00000000 3
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 4
HO2W J 9/78H 1.0 2. 0. 0. G 300.000 5000.000 33.00669 1
0.40173060E 01 0.22175883E-02-0.57710171E-06 0.71372882E-10-0.36458591E-14 2
-0.11412445E 04 0.37846051E 01 0.35964102E 01 0.52500748E-03 0.75118344E-05 3
-0.95674952E-08 0.36597628E-11-0.89333502E 03 0.66372671E 01 0.00000000 4
H2O2W L 3/85H 2.0 2. 0. 0. G 300.000 5000.000 34.01460 1
0.47928858E 01 0.36300865E-02-0.11136435E-05 0.14868513E-09-0.68958511E-14 2
-0.18132195E 05-0.51306415E 00 0.34546633E 01 0.55575930E-02 0.92103738E-06 3
-0.46279780E-08 0.21458200E-11-0.17672328E 05 0.68402452E 01-0.16394994E 05 4
SPECA L 5/66A 1.00 0.00 0.00 0.0 G 300.000 5000.000 0.999001E-03 1
0.25161474E 01 0.00000000 0.00000000 0.00000000 0.00000000 2
0.00000000 0.00000000 0.25161474E 01 0.00000000 0.00000000 3
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 4
SPECB L 5/66A 1.00 0.00 0.00 0.0 G 300.000 5000.000 0.999001E-03 1
0.25161474E 01 0.00000000 0.00000000 0.00000000 0.00000000 2
0.00000000 0.00000000 0.25161474E 01 0.00000000 0.00000000 3
0.00000000 0.00000000 0.00000000 0.00000000 0.00000000 4
END
SIMPLE TEST CASE A=B: HWANG, JT, PROC. NSC TAIWAN, PART B, V6, P37, 1982. CASE 1
SPECA > SPECB 1.00E+03
SPECB > SPECA 1.00E+00

TIME
&prob rhocon=.true., tcon=.true., sencal=.true., senstd=.true.,
print=1.5E-04,1.0E-03,2.0E-02, &end
&start p=1.0, t=300.0, &end
SPECA 0.999001
SPECB 0.000999
END
&solver emax=1.0E-06, atolsp=0.0, &end
INIT
ALLSP END
SENSVAR
ALLSP END
REAC
&senrxn sensaj=.true., allrxn=.true., &end
FINIS
SIMPLE TEST CASE A=B=C: HWANG ET AL, J. CHEM PHYS, V69, P5180, 1978. CASE 2
NEW
DUMA > DUMB 1.0
DUMB > DUMA 100.0
DUMB > DUMC 100.0
DUMC > DUMB 1.0

TIME
&prob rhocon=.true., tcon=.true., sencal=.true.,
print= 0.1, 2.5, 4.5, &end
&start t=300.0, p=1.0, &end
DUMA 1.00
END
&solver emax=1.0E-6, atolsp=1.0E-8, &end
SENSVAR
ALLSP END
REAC
&senrxn allrxn=.true., sensaj=.true., &end
FINIS

```

TABLE E.1.—Continued.

```

ETHANE PYROLYSIS: KRAMER ET AL, APPL MATH MODELLING, V5, P432, 1981. CASE 3
NEW
      C2H6      +      C2H6      >2.OCH3      1.20E+12      0.0      59218.0
      CH3       >      C2H5      +      CH4      8.01E+08      0.0      11943.0
      C2H5      >      C2H4      +      H        3.00E+11      0.0      34974.0
      H         +      C2H6      >      C2H5      +      H2      1.30E+11      0.0      8982.0
      H         +      H         >      H2        6.99E+13      0.0      0.0

TIME
  &prob rhocon=.true., tcon=.true., sencal=.true.,
    print= 1.0, 20.0, &end
  &start p=0.4507, t=923.0, &end
C2H6      1.0
END
  &solver emax=1.0E-6, atolsp=1.0E-8, &end
INIT
C2H6      TEMP      END
SENSVAR
ALLSP      END
REAC
  &senrxn sensaj=.true., rxnum = 1.0, 2.0, &end
FINIS
CH4-O2-AR SHOCK IGNITION: BONI & PENNER, COMB SCI & TECH, V15, P99, 1977. CASE 4
NEW
      M         +      CH4      >      CH3      +      H        4.337E+07      0.0      0.0
      H         +      CH3      >      CH4      +      M        1.106E+17      0.0      0.0
      OH        +      CH4      >      CH3      +      H2O      2.590E+13      0.0      0.0
      CH3        +      H2O      >      OH       +      CH4      1.048E+11      0.0      0.0
      H          +      CH4      >      CH3      +      H2       1.988E+13      0.0      0.0
      CH3        +      H2       >      H        +      CH4      8.071E+11      0.0      0.0
      O          +      CH4      >      CH3      +      OH       2.168E+12      0.0      0.0
      CH3        +      OH       >      O        +      CH4      6.625E+10      0.0      0.0
      CH3        +      O        >      CH2O      +      H        1.0E+14      0.0      0.0
      CH2O       +      H        >      CH3      +      O        5.3E+07      0.0      0.0
      CH3        +      O2       >      CH2O      +      OH       2.0E+10      0.0      0.0
      CH2O       +      OH       >      CH3      +      O2       4.337E+04      0.0      0.0
      CH2O       +      O        >      HCO       +      OH       1.584E+13      0.0      0.0
      HCO        +      OH       >      CH2O      +      O        9.035E+09      0.0      0.0
      CH2O       +      OH       >      HCO       +      H2O      1.108E+14      0.0      0.0
      HCO        +      H2O      >      CH2O      +      OH       8.553E+09      0.0      0.0
      CH2O       +      H        >      HCO       +      H2       5.240E+12      0.0      0.0
      HCO        +      H2       >      CH2O      +      H        4.216E+09      0.0      0.0
      M          +      CH2O     >      HCO       +      H        3.843E+08      0.0      0.0
      HCO        +      H        >      CH2O      +      M        1.959E+16      0.0      0.0
      HCO        +      O        >      CO        +      OH       1.0E+14      0.0      0.0
      CO         +      OH       >      HCO       +      O        1.144E+05      0.0      0.0
      HCO        +      OH       >      CO        +      H2O      1.0E+14      0.0      0.0
      CO         +      H2O      >      HCO       +      OH       1.265E+04      0.0      0.0
      HCO        +      H        >      CO        +      H2       2.0E+14      0.0      0.0
      CO         +      H2       >      HCO       +      H        2.771E+05      0.0      0.0
      M          +      HCO      >      H        +      CO       4.216E+10      0.0      0.0
      H          +      CO       >      HCO       +      M        3.628E+12      0.0      0.0
      CO         +      OH       >      CO2       +      H        5.360E+11      0.0      0.0
      CO2        +      H        >      CO        +      OH       2.289E+11      0.0      0.0
      H2         +      OH       >      H2O      +      H        1.807E+13      0.0      0.0
      H2O        +      H        >      H2       +      OH       1.807E+12      0.0      0.0
      O          +      H2       >      OH       +      H        7.228E+12      0.0      0.0
      OH         +      H        >      O        +      H2       6.625E+12      0.0      0.0
      H          +      O2       >      OH       +      O        3.216E+12      0.0      0.0
      OH         +      O        >      H        +      O2       1.385E+13      0.0      0.0
      H          +      OH       >      H2O      +      M        2.104E+15      0.0      0.0
THIRDBODY
H2O      16.7      END
      M         +      H2O      >      H        +      OH       3.096E+03      0.0      0.0
THIRDBODY
H2O      16.7      END
      H         +      HO2      >2.OOH      1.554E+14      0.0      0.0
      H         +      2.OOH     >      H        +      HO2      6.023E+08      0.0      0.0
      H         +      O2       >      HO2      +      M        1.930E+15      0.0      0.0
      M         +      HO2      >      H        +      O2       2.168E+10      0.0      0.0
      OH        +      OH       >      O        +      H2O      9.456E+12      0.0      0.0
      O         +      H2O      >      OH       +      OH       1.205E+12      0.0      0.0

AR
TIME
  &prob rhocon=.true., tcon=.true., sencal=.true., print= 2.5E-5,
    &end
  &start t=2000.0, p=6.729, &end
CH4      0.09172
O2       0.18344
AR       0.72484

```

TABLE E.1.—Continued.

```

CO2          4.0494E-20
H2           4.0494E-20
END
&solver mf=21, emax=1.0E-3, atolsp=1.0E-12, &end
SENSVAR
ALLSP      END
REAC
&senrxn sensaj=.true., allrxn=.true., &end
FINIS
FORMALDEHYDE OXID.: DOUGHERTY ET AL, J. CHEM PHYS, V71, P1794, 1979.      CASE 5
NEW
HCO + O2 > CO + HO2 6.02E+10 0. 0.
HO2 + CH2O > H2O2 + HCO 3.43E+10 0. 0.
M + H2O2 > 2.0OH 4.01E+06 0. 0.
CH2O + OH > HCO + H2O 9.64E+13 0. 0.
OH + H2O2 > H2O + HO2 3.07E+12 0. 0.
H2O2 > H2O2W 1.05E+2 0. 0.
HO2 > HO2W 1.05E+1 0. 0.
HO2 + HO2 > H2O2 + O2 1.81E+12 0. 0.
CO + OH > CO2 + H 1.99E+11 0. 0.
CO + HO2 > CO2 + OH 7.23E+08 0. 0.
CH2O + H > HCO + H2 1.63E+12 0. 0.
H + O2 > OH + O 3.32E+10 0. 0.
H + O2 > HO2 + M 3.63E+15 0. 0.
M + HO2 > H + O2 2.83E+05 0. 0.
O + H2 > OH + H 1.82E+11 0. 0.
CH2O + O > HCO + OH 6.02E+13 0. 0.
H + H2O2 > HO2 + H2 7.83E+11 0. 0.
H + H2O2 > H2O + OH 3.55E+12 0. 0.
O + H2O2 > OH + HO2 6.02E+10 0. 0.
HCO > H + CO 4.60E-12 0. 0.
H2 + OH > H2O + H 6.02E+12 0. 0.
CH2O + O2 > HCO + HO2 1.75E+04 0. 0.
H + HO2 > 2.0OH 3.01E+12 0. 0.
HO2 + H > H2O + O 3.01E+13 0. 0.
H + HO2 > H2 + O2 2.71E+13 0. 0.

N2
TIME
&prob rhocon=.true., tcon=.true., sencal=.true., tiny=0.1,
print= 1.0E-06,5.0E-03, &end
&start t=952.0, p=0.918066, &end
CH2O 0.009564
CO 0.399833
O2 0.179453
N2 0.411150
END
&solver emax=1.0E-06, atolsp=1.0E-08, &end
SENSVAR
ALLSP      END
REAC
&senrxn allrxn=.true., sensaj=.true., order=.true., &end
FINIS
WET CO OXIDATION: YETTER ET AL, COMB & FLAME, V59, P107, 1985.      CASE 6
NEW
HCO + H > CO + H2 2.0E+14 0. 0.
CO + H2 > HCO + H 1.716E-3 0. 0.
HCO + OH > CO + H2O 1.0E+14 0. 0.
CO + H2O > HCO + OH 3.656E-06 0. 0.
HCO + O > CO + OH 3.012E+13 0. 0.
CO + OH > O + HCO 2.867E-04 0. 0.
HCO + O2 > CO + HO2 3.015E+12 0. 0.
CO + HO2 > HCO + O2 2.590E+06 0. 0.
CO + HO2 > CO2 + OH 3.084E+09 0. 0.
CO2 + OH > CO + HO2 1.777E-02 0. 0.0
CO + OH > CO2 + H 1.921E+11 0. 0.
CO2 + H > CO + OH 7.890E+08 0.0 0.0
CO2 + O > CO + O2 4.434E+02 0. 0.
CO + O2 > CO2 + O 8.492E+02 0. 0.0
H + O2 > OH + O 1.126E+11 0. 0.
OH + O > H + O2 1.385E+13 0. 0.0
O + H2 > OH + H 3.385E+11 0. 0.
OH + H > O + H2 3.831E+11 0.0 0.0
O + H2O > OH + OH 1.650E+10 0. 0.
OH + OH > O + H2O 4.108E+12 0. 0.0
H2O + H > OH + H2 7.709E+09 0. 0.
OH + H2 > H2O + H 1.837E+12 0. 0.0
OH + H2O2 > H2O + HO2 3.632E+12 0. 0.
H2O + HO2 > OH + H2O2 7.107E+06 0. 0.0
O + HO2 > OH + O2 2.168E+13 0. 0.
OH + O2 > O + HO2 2.475E+02 0. 0.0
H + HO2 > 2.0OH 1.126E+14 0. 0.0

```

TABLE E.1.—Continued.

```

OH      + OH      > H      + HO2      1.385E+05  0.      0.0
H      + HO2      > H2     + O2      2.506E+13  0.      0.0
H2     + O2      > H      + HO2      2.487E+02  0.      0.0
HO2    + OH      > H2O    + O2      1.313E+13  0.      0.0
H2O    + O2      > HO2    + OH      5.529E-01  0.      0.0
O2     + H2O2    > 2.OHO2  1.349E+05  0.      0.0
HO2    + HO2     > O2     + H2O2    6.324E+12  0.      0.0
HO2    + H2      > H2O2   + H      1.403E+08  0.      0.
H2O2   + H      > HO2    + H2      3.054E+11  0.      0.0
M      + O2      > O      + O      2.030E-08  0.      0.
O      + O      > O2     + M      1.861E+14  0.      0.0
M      + H2      > H      + H      1.850E-05  0.      0.
H      + H      > H2     + M      3.000E+15  0.      0.0
M      + OH      > O      + H      1.807E-04  0.      0.
O      + H      > OH     + M      1.001E+16  0.      0.0
M      + H2O2    > 2.OOH   1.090E+08  0.      0.
OH     + OH      > H2O2   + M      9.251E+15  0.      0.0
M      + H2O     > H      + OH      3.012E-05  0.0    0.
H      + OH      > H2O    + M      1.157E+17  0.0    0.0
M      + HO2     > H      + O2      1.753E+06  0.      0.
H      + O2      > HO2    + M      2.605E+15  0.      0.0
M      + CO2     > CO      + O      3.234E-08  0.      0.
CO     + O      > CO2    + M      9.069E+14  0.0    0.0
M      + HCO     > H      + CO      2.777E+10  0.      0.
H      + CO      > HCO    + M      3.210E+14  0.      0.0

N2
TIME
&prob rhocon=.true., tcon=.true., sencal=.true.,
      print=1.0E-4,1.0E-1,1.0E2, &end
&start t=1100.0, p=1.0, &end
CO      0.002
H2O     0.01
O2      0.028
N2      0.96
END
&solver emax=1.0E-3, atolsp=1.0E-12, &end
SENSVAR
CO      H2
END
INIT
HCO     H      OH      O      HO2     H2O2     END
REAC
&senrxn sensaj=.true., allrxn=.true., output=.false., order=.true.,
&end
FINIS
SIMPLE NONISOTHERMAL TEST CASE R>P CASE 7
NEW
DUMR    > DUMP      1.0  1.0  0.0

TIME      PRESSURE
&prob pcon=.true., sencal=.true., senstd=.true.,
      print=1.0E-06,1.0E-04,1.0E-02, &end
&start t=1000.0, p=1.0, &end
DUMR     1.00
END
&solver emax=1.0E-3, atolsp=1.0E-12, &end
INIT
ALL      END
SENSVAR
ALL      END
REAC
&senrxn sensaj=.true., sensnj=.true., sensej=.true., allrxn=.true.,
&end
FINIS
HYDROGEN COMBUSTION IN STANDARD AIR AT 3.10 ATM CASE 8
NEW
CO      + O      = CO2    + M      5.888E+15  0.      4100.
CO      + O2     = CO2    + O      2.512E+12  0.      47690.
CO      + OH     = CO2    + H      4.169E+11  0.      1000.
CO      + HO2    = CO2    + OH     5.754E+13  0.      22930.
O      + H2O     = OH     + OH     6.8E+13  0.0    18365.
H      + O2     = OH     + O      1.89E+14  0.      16400.
O      + H2     = OH     + H      4.20E+14  0.      13750.
H      + HO2    = H2     + O2     7.28E+13  0.      2126.
O      + HO2    = OH     + O2     5.0E+13  0.      1000.
HO2    + OH     = H2O    + O2     8.0E+12  0.      0.
H      + HO2    = 2.OOH   1.34E+14  0.      1070.
H2     + HO2    = H2O2   + H      7.91E+13  0.      25000.
OH     + H2O2    = H2O    + HO2    6.1E+12  0.      1430.
HO2    + HO2    = H2O2   + O2     1.8E+12  0.      0.

```


TABLE E.1.—Continued.

H	+	H2O2	=	OH	+	H2O	7.8E+11	0.	0.
M	+	H2O2	=	2.OOH			1.44E+17	0.	45510.
THIRDBODY									
H2		2.30	O2		.78	H2O	6.0	H2O2	6.6
END									
H2	+	OH	=	H2O	+	H	4.74E+13	0.	6098.
H	+	O2	=	HO2	+	M	1.46E+15	0.	-1000.
THIRDBODY									
O2		1.30	N2		1.3	H2O	21.3	H2	5.0
END									
M	+	H2O	=	H	+	OH	1.30E+15	0.	105140.
THIRDBODY									
H2		4.00	O2		1.5	H2O	20.0	N2	1.5
END									
H	+	O	=	OH	+	M	7.1E+18	-1.	0.
M	+	H2	=	H	+	H	2.2E+14	0.	96000.
THIRDBODY									
H2		4.10	O2		2.0	H2O	15.0	N2	2.0
END									
M	+	O2	=	O	+	O	1.80E+18	-1.	118020.
HO2	+	NO	=	NO2	+	OH	2.09E+12	0.0	-477.
O	+	NO2	=	NO	+	O2	1.0E+13	0.0	596.
NO	+	O	=	NO2	+	M	5.62E+15	0.	-1160.
NO2	+	H	=	NO	+	OH	3.47E+14	0.	1470.
NO	+	O	=	N	+	O2	3.8E+9	1.0	41370.
O	+	N2	=	NO	+	N	1.8E+14	0.	76250.
NO	+	H	=	N	+	OH	2.63E+14	0.	50410.
M	+	N2O	=	N2	+	O	6.92E+23	-2.5	65000.
O	+	N2O	=	N2	+	O2	1.0E+14	0.	28020.
O	+	N2O	=	2.0NO			6.92E+13	0.	26630.
N	+	NO2	=	2.0NO			4.0E+12	0.	0.0
N2O	+	H	=	N2	+	OH	7.59E+13	0.	15100.
NO2	+	H2	=	HNO2	+	H	2.4E+13	0.	29000.
OH	+	NO2	=	HNO3	+	M	3.0E+15	0.	-3800.
THIRDBODY									
O2		0.70	H2		1.4	END	5.6E+15	0.	-1700.
OH	+	NO	=	HNO2	+	M	5.0E+12	0.	0.
HNO	+	H	=	H2	+	NO	5.4E+15	0.	-600.
H	+	NO	=	HNO	+	M	3.6E+13	0.	0.
HNO	+	OH	=	H2O	+	NO			

AR

TIME PRESSURE

```
&prob sencal=.true., tiny=1.0E-7,
print= 1.0E-4, 1.8E-4, 2.0E-4, ct0=3.1, &end
&start t= 950.66, &end
```

```
H2 0.2952726
O2 0.1476404
CO2 2.1140E-4
N2 0.5458075
NO 0.0045
AR 6.5681E-3
END
```

```
&solver emax= 1.0E-4, atolsp= 1.0E-13, &end
```

```
INIT CO H2 O2 HO2 H2O2 NO TEMP DENSITY
```

REAC

```
&senrxn sensaj=.true., sensej=.true., output=.false., order=.true.,
rxnum=5.0,6.0,8.0,11.0,17.0,18.0, &end
```

```
SENSVAR CO CO2 OH H2O H2 NO TEMP END
```

FINIS BENZENE-OXYGEN-AR SHOCK IGNITION - WITH SENSITIVITY MECHANISM K-70 CASE 9

NEW

C6H6	+	O2	=	C6H5O	+	OH	4.0E+13	0.	34000.
C6H6	+	C6H5	=	C12H10	+	H	4.0E+11	0.	4000.
		C6H6	=	C6H5	+	H	1.0E+16	0.	108000.
C6H6	+	H	=	C6H5	+	H2	2.5E+14	0.	16000.
C6H6	+	O	=	C6H5O	+	H	2.783E+13	0.	4910.
C6H6	+	OH	=	C6H5	+	H2O	2.132E+13	0.	4580.
M	+	C4H3	=	C4H2	+	H	1.0E+16	0.0	60000.
		C6H5O	=	C5H5	+	CO	2.51E+11	0.	43900.
C6H5	+	O2	=	C6H5O	+	O	2.1E+12	0.	7470.
C6H5	+	HO2	=	C6H5O	+	OH	2.0E+13	0.	1000.
		C6H5	=	C4H3	+	C2H2	4.50E+13	0.	72530.
		C6H5OH	=	C6H5O	+	H	2.00E+16	0.	88000.
C6H5OH	+	H	=	C6H6	+	OH	2.20E+13	0.	7910.
C6H5OH	+	H	=	C6H5O	+	H2	1.15E+14	0.	12405.
C5H5	+	C6H5OH	=	C6H5O	+	C5H6	2.67E+14	0.	25227.
		C5H6	=	C5H5	+	H	8.13E+24	-2.981	78682.
C5H6	+	O2	=	C5H5O	+	OH	1.0E+13	0.	20712.

TABLE E.1.—Continued.

C6H5OH	+	OH	=	C6H5O	+	H2O	3.0E+13	0.	0.
C6H5OH	+	HO2	=	C6H5O	+	H2O2	3.0E+13	0.	1500.
		C5H5O	=	C4H5	+	CO	3.0E+16	0.	15000.
C5H5	+	O	=	C5H5O			1.0E+13	0.	0.
C5H5	+	OH	=	C5H4OH	+	H	1.0E+13	0.	0.
		C5H4OH	=	C4H4	+	HCO	1.0E+15	0.	22000.
C5H5	+	HO2	=	C5H5O	+	OH	2.0E+13	0.	0.
	2.0C6H5		=	C12H10			3.1E+12	0.	0.
	C4H5		=	C2H3	+	C2H2	1.4E+13	0.	32900.
C4H2	+	O	=	C2HO	+	C2H	1.0E+13	0.	0.
C4H2	+	OH	=	HCO	+	C3H2	3.0E+13	0.	0.
C4H2	+	O	=	CO	+	C3H2	1.2E+12	0.	0.
M	+	C2H4	=	C2H2	+	H2	9.33E+16	0.	77200.
C2H4	+	OH	=	C2H3	+	H2O	4.786E+12	0.	1230.
C2H4	+	O	=	CH3	+	HCO	3.311E+12	0.	1130.
C2H4	+	O	=	CH2O	+	CH2	2.512E+13	0.	5000.
C2H4	+	OH	=	CH3	+	CH2O	1.995E+12	0.	960.
M	+	C2H3	=	C2H2	+	H	3.0E+15	0.	32000.
C2H3	+	O2	=	CH2O	+	HCO	3.98E+12	0.	-250.
C2H3	+	H	=	C2H2	+	H2	6.0E+12	0.	0.
C2H3	+	OH	=	C2H2	+	H2O	5.012E+12	0.	0.
C2H3	+	CH2	=	C2H2	+	CH3	3.020E+13	0.	0.
C2H3	+	C2H	=	2.0C2H2			3.020E+13	0.	0.
C2H3	+	O	=	C2H2O	+	H	3.3E+13	0.	0.
CH2	+	CH2	=	C2H2	+	H2	4.0E+13	0.	0.
CH2	+	CH2	=	C2H3	+	H	5.012E+12	0.	0.
CH2	+	OH	=	CH	+	H2O	2.51E+11	.67	25700.
CH2	+	O	=	CH	+	OH	2.0E+11	.68	25000.
CH2	+	O2	=	CO2	+	2.0H	1.59E+12	0.	1000.
M	+	C2H2	=	C2H	+	H	4.169E+16	0.	107000.
C2H2	+	C2H2	=	C4H3	+	H	2.0E+12	0.	45900.
C2H2	+	O	=	CH2	+	CO	1.6E+14	0.0	9890.
C2H2	+	O	=	C2HO	+	H	4.0E+14	0.0	10660.
C2H2	+	OH	=	C2H	+	H2O	6.310E+12	0.	7000.
C2H2	+	OH	=	C2H2O	+	H	3.2E+11	0.	200.
C2H2	+	C2H	=	C4H2	+	H	3.0E+13	0.	0.
C2H2	+	CH2	=	C3H3	+	H	1.2E+13	0.	6600.
M	+	C3H4	=	C3H3	+	H	2.0E+17	0.	65000.
C2H2O	+	OH	=	CH2O	+	HCO	2.8E+13	0.	0.
C2H2O	+	OH	=	C2HO	+	H2O	7.5E+12	0.	3000.
C2H2O	+	H	=	CH3	+	CO	1.13E+13	0.	3428.
C2H2O	+	H	=	C2HO	+	H2	7.5E+13	0.	8000.
C2H2O	+	O	=	C2HO	+	OH	5.0E+13	0.	8000.
C2H2O	+	O	=	CH2O	+	CO	2.0E+13	0.	0.
M	+	C2H2O	=	CH2	+	CO	2.0E+16	0.	60000.
C2HO	+	O2	=	2.0CO	+	OH	1.46E+12	0.	2500.
C2HO	+	O	=	2.0CO	+	H	1.202E+12	0.	0.
C2HO	+	OH	=	2.0HCO			1.0E+13	0.	0.
C2HO	+	H	=	CH2	+	CO	5.0E+13	0.	0.
C2HO	+	CH2	=	C2H3	+	CO	3.0E+13	0.	0.
C2HO	+	CH2	=	CH2O	+	C2H	1.0E+13	0.	2000.
	2.0C2HO		=	C2H2	+	2.0CO	1.0E+13	0.	0.
C2H	+	OH	=	C2HO	+	H	2.0E+13	0.	0.
C2H	+	O2	=	C2HO	+	O	5.00E+13	0.	1500.
C2H	+	O	=	CO	+	CH	5.012E+13	0.	0.
M	+	CH4	=	CH3	+	H	2.0E+17	0.	88000.
CH4	+	O2	=	CH3	+	HO2	7.943E+13	0.	56000.
CH4	+	H	=	CH3	+	H2	1.26E+14	0.	11900.
OH	+	CH4	=	CH3	+	H2O	2.5E+13	0.	5010.
O	+	CH4	=	CH3	+	OH	1.9E+14	0.	11720.
CH3	+	O2	=	CH3O	+	O	4.786E+13	0.	29000.
CH3	+	OH	=	CH3O	+	H	6.3E+12	0.	0.
M	+	CH3O	=	CH2O	+	H	5.0E+13	0.	21000.
CH3O	+	O2	=	CH2O	+	HO2	1.0E+12	0.	6000.
CH3O	+	H	=	CH2O	+	H2	2.0E+13	0.	0.
CH3	+	CH3	=	C2H4	+	H2	1.0E+16	0.	32000.
CH3	+	O	=	CH2O	+	H	1.288E+14	0.	2000.
CH3	+	CH2O	=	CH4	+	HCO	1.0E+10	0.5	6000.
CH3	+	HCO	=	CH4	+	CO	3.020E+11	.5	0.
CH3	+	HO2	=	CH3O	+	OH	2.00E+13	0.	0.
M	+	CH2O	=	HCO	+	H	5.0E+16	0.	81000.
CH2O	+	OH	=	HCO	+	H2O	3.0E+13	0.	1200.
CH2O	+	H	=	HCO	+	H2	2.5E+13	0.	3990.
CH2O	+	O	=	HCO	+	OH	3.5E+13	0.	3510.
HCO	+	HO2	=	CH2O	+	O2	1.0E+14	0.	3000.
M	+	HCO	=	H	+	CO	2.94E+14	0.	15569.
HCO	+	O2	=	CO	+	HO2	3.311E+12	0.	7000.
HCO	+	OH	=	CO	+	H2O	1.0E+14	0.	0.
HCO	+	H	=	CO	+	H2	1.995E+14	0.	0.
HCO	+	O	=	CO	+	OH	1.0E+14	0.	0.
CH	+	O2	=	HCO	+	O	1.0E+13	0.	0.
CO	+	O	=	CO2	+	M	5.9E+15	0.	4100.

TABLE E.1.—Concluded.

```

CO      +   O2      =   CO2      +   O          2.5E+12   0.      47690.
CO      +   OH       =   CO2      +   H          4.17E+11   0.      1000.
CO      +   HO2      =   CO2      +   OH         5.75E+13   0.      22930.
O       +   H2O      =   OH       +   OH         6.8E+13   0.      18365.
H       +   O2       =   OH       +   O          1.89E+14   0.      16400.
O       +   H2       =   OH       +   H          4.20E+14   0.      13750.
H       +   HO2      =   H2       +   O2         7.28E+13   0.      2126.
O       +   HO2      =   OH       +   O2         5.0E+13   0.      1000.
HO2     +   OH       =   H2O      +   O2         8.0E+12   0.      0.
H       +   HO2      =2.0OH          1.34E+14   0.      1070.
H2      +   HO2      =   H2O2     +   H          7.91E+13   0.      25000.
OH      +   H2O2     =   H2O      +   HO2         6.1E+12   0.      1430.
HO2     +   HO2      =   H2O2     +   O2         1.8E+12   0.      0.
H       +   H2O2     =   OH       +   H2O         7.8E+11   0.      0.
M       +   H2O2     =   OH       +   OH         1.44E+17   0.      45510.
THIRDBODY
H2      2.30      O2      .78      H2O      6.0      H2O2      6.6
END
H2      +   OH       =   H2O      +   H          4.74E+13   0.      6098.
H       +   O2       =   HO2      +   M          1.46E+15   0.      -1000.
THIRDBODY
O2      1.30      CO2      7.0      H2O      21.3      H2      3.0
C6H6    20.0      CH4      5.0      END
M       +   H2O      =   H       +   OH          1.30E+15   0.      105140.
THIRDBODY
H2      4.00      O2      1.5      H2O      20.0      C6H6      20.0
CO2     4.00      END
H       +   O       =   OH       +   M          7.1E+18   -1.      0.
M       +   H2      =   H       +   H          2.2E+14   0.      96000.
THIRDBODY
H2      4.10      O2      2.0      H2O      15.0      END
M       +   O2      =   O       +   O          1.80E+18   -1.      118020.

AR
TIME
&prob   iprint=50, rhocon=.true., sencal=.true., tiny=1.0E-7,
&end=3.07E-4, &end
&start  t= 1405.0, p=2.3868, &end
C6H6    0.01690
O2      0.12582
AR      0.85728
END
&solver  emax= 1.0E-4, atolsp= 1.0E-13, &end
SENSVAR
C6H6    C6H5      H2O      CO      C2H2      C6H5OH      C5H6      TEMP
DENSITY PRESSURE  END
INIT
C6H6    OH      AR      TEMP      DENSITY  END
REAC
&senrxn sensaj=.true., sensej=.true.,
rxnum=1.0,2.0,3.0,4.0,5.0,6.0,7.0,8.0,10.0,11.0,12.0,13.0,
14.0,15.0,16.0,17.0,18.0,19.0,20.0,21.0,101.0,104.0,116.0, &end
FINIS

```

TABLE E.2.—SELECTED SENSITIVITY TEST CASE RESULTS
(a) Case 1

[illegible]

*** THE FOLLOWING 1 ELEMENTS CONSIDERED FOR THIS PROBLEM ***

A

*** THE FOLLOWING 2 REACTING SPECIES CONSIDERED FOR THIS PROBLEM ***

SPECA SPECB

*** NO INERT SPECIES CONSIDERED FOR THIS PROBLEM ***

*** THERMODYNAMIC DATA, MOLECULAR WEIGHT AND HEAT OF FORMATION AT 25 C ***

SPECA		MHT = 0.00099900		H(25 C) = 1.4907E+01 CAL/MOLE	
0.25161474E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00
0.25161474E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00

SPECB		MHT = 0.00099900		H(25 C) = 1.4907E+01 CAL/MOLE	
0.25161474E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00
0.25161474E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM

NASA LENS RESEARCH CENTER

SIMPLE TEST CASE A=B; HNAIG, JT, PROC. NSC TAIWAN, PART B V6, P57, 1982. CASE 1

REACTION NUMBER	REACTION		REACTION RATE A	VARIABLES N	ACTIVATION ENERGY
1	1#SPECA	> 1#SPECB	1.00000E+03	0.0000	0.00
2	1#SPECB	> 1#SPECA	1.00000E+00	0.0000	0.00

TABLE E.2.—Continued.
(a) Continued.

```

** INPUT DATA GIVEN IN CGS UNITS **                ** OUTPUT REQUIRED IN CGS UNITS **

** ASSIGNED VARIABLE PROFILE **

THIS IS A CONSTANT DENSITY PROBLEM - AN ASSIGNED VARIABLE IS NOT REQUIRED

THE TEMPERATURE WILL BE HELD CONSTANT FOR THIS CASE

NUMBER OF REACTING SPECIES:    2
NUMBER OF INERT SPECIES:      0

NUMBER OF SPECIES ODE'S REQUIRED FOR THIS CASE:    2
TOTAL NUMBER OF ODE'S REQUIRED FOR THIS CASE:    2

INTEGRATION CONTROLS
INTEGRATION METHOD (MF):  21      MAXIMUM RELATIVE ERROR:  1.00000E-06      SPECIES ABSOLUTE ERROR:  0.00000E+00
MAXIMUM NUMBER OF STEPS ALLOWED FOR THE COMPLETE PROBLEM:  2000

**** SENSITIVITY ANALYSIS REQUIRED ****

*** SENSITIVITY OF FOLLOWING  2 VARIABLES WILL BE CALCULATED ***
SPECA    SPECB

*** SENSITIVITY WRT INITIAL VALUES OF FOLLOWING  2 VARIABLES REQUIRED ***
SPECA    SPECB

*** CONSTANT TEMPERATURE CASE SO SENSITIVITY COEFFICIENTS WRT ONLY PREEXPONENTIAL FACTORS WILL BE CALCULATED ***
NORMALIZATION FACTOR FOR AJ = AJ

** SENSITIVITY COEFFICIENTS WRT RATE CONSTANT PARAMETERS REQUIRED FOR FOLLOWING  2 REACTIONS **

1    2

*** SENSITIVITY COEFFICIENTS OF FIRST-ORDER TIME DERIVATIVES ALSO REQUIRED ***

** OUTPUT REQUIRED AT FOLLOWING  5 PRINT STATIONS **

STATION      TIME (SEC)
1            1.50000E-04
2            1.00000E-03
3            2.00000E-02

```

TABLE E.2.—Continued.
(a) Continued.

** INITIAL CONDITIONS **									
TIME	0.00000E+00	SEC	AREA	0.00000E+00	SQ CM	AXIAL POSITION	0.00000E+00	CM	
FLOW PROPERTIES					INTEGRATION INDICATORS				
PRESSURE (ATM)	1.00000		STEPS FROM LAST PRINT		0				
VELOCITY (CM/SEC)	0.00		AVERAGE STEP SIZE		0.00000E+00				
DENSITY (G/CM**3)	4.05821E-08		METHOD ORDER		0				
TEMPERATURE (DEG K)	300.00								
MASS FLOW RATE (G/SEC)	0.00000E+00		TOTAL NUMBER OF STEPS		0				
ENTROPY (CAL/G/DEG K)	28563.1484		FUNCT EVALUATIONS		0				
MACH NUMBER	0.0000		JACOBIAN EVALUATIONS		0				
GAMMA	1.6596								
ENTHALPY (CAL/G)	1.50150E+06								
SP. HEAT (CP) (CAL/G/DEG K)	5.00500E+03								
CHEMICAL PROPERTIES									
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE		
SPECA	4.05821E-05	9.99001E-01	-4.05820E-02	1	1.0000E+03	2.46414E+15	1.00000		
SPECB	4.05820E-08	9.99000E-04	-4.05820E-02	2	1.0000E+00	2.46414E+07	1.00000		
DERIVATIVES (CGS UNITS): T			0.00000E+00	RHO	0.00000E+00				
MIXTURE MOLECULAR WEIGHT	0.00100		TOTAL ENERGY EXCHANGE RATE (CAL CM**3/G**2/SEC)	0.0000E+00	MASS FRACTION SUM	1.00000000			
CPU TIME FOR INITIALIZATION OF LSENS = 0.491000 S									

TIME	2.00000E-02	SEC	AREA	0.00000E+00	SQ CM	AXIAL POSITION	0.00000E+00	CM	
FLOW PROPERTIES					INTEGRATION INDICATORS				
PRESSURE (ATM)	1.00000		STEPS FROM LAST PRINT		105				
VELOCITY (CM/SEC)	0.00		AVERAGE STEP SIZE		0.18141E-03				
DENSITY (G/CM**3)	4.05821E-08		METHOD ORDER		5				
TEMPERATURE (DEG K)	300.00								
MASS FLOW RATE (G/SEC)	0.00000E+00		TOTAL NUMBER OF STEPS		135				
ENTROPY (CAL/G/DEG K)	28563.1484		FUNCT EVALUATIONS		155				
MACH NUMBER	0.0000		JACOBIAN EVALUATIONS		15				
GAMMA	1.6596								
ENTHALPY (CAL/G)	1.50150E+06								
SP. HEAT (CP) (CAL/G/DEG K)	5.00500E+03								
CHEMICAL PROPERTIES									
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE		
SPECA	4.05822E-08	9.99004E-04	-3.04065E-10	1	1.0000E+03	2.46415E+10	1.00000		
SPECB	4.05821E-05	9.99001E-01	1.04065E-10	2	1.0000E+00	2.46414E+10	1.00000		
DERIVATIVES (CGS UNITS): T			0.00000E+00	RHO	0.00000E+00				
MIXTURE MOLECULAR WEIGHT	0.00100		TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	0.00000E+00	MASS FRACTION SUM	1.00000000			

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 2.000000E-01 S UP TO THIS TIME - 2.599999E-01 S

TABLE E.2.—Continued.

(a) Concluded.

```

***** SENSITIVITY CALCULATIONS *****
TIME = 2.00000D-02
SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

***** SENSITIVITY TO INITIAL CONDITIONS *****
DZ(I)/DYZERO(J)*F(J)/Z(I), WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
F(J)= YZERO(J) FOR YZERO(J) NOT EQUAL TO 0
      = 1.0E-4/(INITIAL MNT) FOR YZERO(J) = 0

PARAMETER   SPECA   SPECB
SPECA       9.990D-01 9.990D-01
SPECB       9.990D-04 9.990D-04

***** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS *****
DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
***** NOTE: FOR CONSTANT TEMPERATURE PROBLEMS NORMALIZED SENSITIVITY COEFFICIENTS W.R.T. H(J) AND E(J) ARE
THE SAME AS THE NORMALIZED COEFFICIENTS W.R.T. A(J) *****

REAC NUM     SPECA   SPECB
1            -9.990D-01 9.990D-04
2            9.990D-01 -9.990D-04

***** SENSITIVITY CALCULATIONS *****
TIME = 2.00000D-02
SENSITIVITY COEFFICIENTS OF 1-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

***** SENSITIVITY TO INITIAL CONDITIONS *****
DZ(I)/DYZERO(J)*F(J)/Z(I), WHERE Z(I)= 1-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
F(J)= YZERO(J) FOR YZERO(J) NOT EQUAL TO 0
      = 1.0E-4/(INITIAL MNT) FOR YZERO(J) = 0

PARAMETER   SPECA   SPECB
SPECA       9.972D-01 9.972D-01
SPECB      -9.972D-07 -9.972D-07

***** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS *****
DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 1-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
***** NOTE: FOR CONSTANT TEMPERATURE PROBLEMS NORMALIZED SENSITIVITY COEFFICIENTS W.R.T. H(J) AND E(J) ARE
THE SAME AS THE NORMALIZED COEFFICIENTS W.R.T. A(J) *****

REAC NUM     SPECA   SPECB
1            -1.808D+01 -1.808D+01
2            -1.908D-02 -1.908D-02

(LSENS)      END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:
TOTAL NO. OF STEPS - 135
TOTAL NO. OF DERIVATIVE EVALUATIONS - 133
TOTAL NO. OF JACOBIAN EVALUATIONS - 15
TOTAL CPU TIME - 0.260000 S

WORK REQUIRED BY SENSITIVITY ROUTINE:
NO. STEPS = 135
NO. FUNC. EVAL. = 135
NO. JAC. EVAL. = 135
TOTAL REAL SPACE USED = 100
TOTAL INTEGER SPACE USED = 44

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 0.920000 S

(LSENS)      READ DATA FOR NEXT CASE

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TABLE E.2.—Continued.
(b) Case 2

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM				NASA LEWIS RESEARCH CENTER			
SIMPLE TEST CASE A=B=C; HUANG ET AL, J. CHEM PHYS, V69, P180, 1978.				CASE 2			
REACTION NUMBER	REACTION			REACTION RATE VARIABLES		ACTIVATION ENERGY	
	A		B	A	B		
1	1*DUMA	>	1*DUMB	1.00000E+00	0.0000	0.00	
2	1*DUMB	>	1*DUMA	1.00000E+02	0.0000	0.00	
3	1*DUMB	>	1*DUMC	1.00000E+02	0.0000	0.00	
4	1*DUMC	>	1*DUMB	1.00000E+00	0.0000	0.00	
** INITIAL CONDITIONS **							
TIME	0.00000E+00	SEC	AREA	0.00000E+00	SQ CM	AXIAL POSITION 0.00000E+00 CM	
FLOW PROPERTIES			INTEGRATION INDICATORS				
PRESSURE (ATM)	1.00000		STEPS FROM LAST PRINT	0			
VELOCITY (CM/SEC)	0.00		AVERAGE STEP SIZE	0.00000E+00			
DENSITY (G/CM**3)	4.06227E-05		METHOD ORDER	0			
TEMPERATURE (DEG K)	300.00		TOTAL NUMBER OF STEPS	0			
MASS FLOW RATE (G/SEC)	0.00000E+00		FUNC1 EVALUATIONS	0			
ENTROPY (CAL/G/DEG K)	28.5189		JACOBIAN EVALUATIONS	0			
MACH NUMBER	0.0000						
GAMMA	1.6596						
ENTHALPY (CAL/G)	1.50000E+03						
SP. HEAT (CP) (CAL/G/DEG K)	5.00000E+00						
CHEMICAL PROPERTIES							
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CJS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POST- TIVE DIR RATE
DUMA	4.06227E-05	1.00000E+00	-4.06227E-05	1	1.0000E+00	2.46168E+04	1.00000
DUMB	0.00000E+00	0.00000E+00	4.06227E-05	2	1.0000E+02	0.00000E+00	0.00000
DUMC	0.00000E+00	0.00000E+00	0.00000E+00	3	1.0000E+02	0.00000E+00	0.00000
				4	1.0000E+00	0.00000E+00	0.00000
DERIVATIVES (CGS UNITS): T			0.00000E+00	RHO	0.00000E+00		
MIXTURE MOLECULAR WEIGHT		1.00000	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)		0.00000E+00	MASS FRACTION SUM	1.00000000
CPU TIME FOR INITIALIZATION OF LSENS = 0.340000 S							

TABLE E.2.—Continued.
(b) Continued.

TIME 2.50000E+00 SEC		AREA 0.00000E+00 SQ CM		AXIAL POSITION 0.00000E+00 CM			
FLOW PROPERTIES				INTEGRATION INDICATORS			
PRESSURE (ATM)	1.00000	STEPS FROM LAST PRINT		50			
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE		0.48681E-01			
DENSITY (G/CM**3)	4.06227E-05	METHOD ORDER		4			
TEMPERATURE (DEG K)	300.00	TOTAL NUMBER OF STEPS		120			
MASS FLOW RATE (G/SEC)	0.00000E+00	FUNCT EVALUATIONS		150			
ENTROPY (CAL/G/DEG K)	29.9450	JACOBIAN EVALUATIONS		19			
MACH NUMBER	0.0000						
GAMMA	1.6596						
ENTHALPY (CAL/G)	1.50000E+03						
SP. HEAT (CP) (CAL/G/DEG K)	5.00000E+00						
CHEMICAL PROPERTIES							
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
DUMA	2.18775E-05	5.38555E-01	-1.66726E-06	1	1.0000E+00	1.32575E+04	1.00000
DUMB	2.02105E-07	4.97512E-03	-4.30623E-13	2	1.0000E+02	1.22472E+04	1.00000
DUMC	1.85430E-05	4.56470E-01	1.66726E-06	3	1.0000E+02	1.22472E+04	1.00000
				4	1.0000E+00	1.12368E+04	1.00000
DERIVATIVES (CGS UNITS): T		0.00000E+00	RHO	0.00000E+00			
MIXTURE MOLECULAR WEIGHT		1.00000	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)		0.00000E+00	MASS FRACTION SUM	1.00000000
COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 1.300000E-01 S UP TO THIS TIME - 3.099999E-01 S							
***** SENSITIVITY CALCULATIONS *****							
TIME = 2.50000E+00							
SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES							
***** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS *****							
DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW							
***** NOTE: FOR CONSTANT TEMPERATURE PROBLEMS NORMALIZED SENSITIVITY COEFFICIENTS W.R.T. H(J) AND E(J) ARE THE SAME AS THE NORMALIZED COEFFICIENTS W.R.T. A(J) *****							
REAC NUM	DUMA	DUMB	DUMC				
1	-5.217D-01	5.388D-01	6.097D-01				
2	-4.261D-01	-4.975D-01	-4.975D-01				
3	-4.215D-01	-4.975D-01	5.027D-01				
4	3.266D-01	4.563D-01	-3.903D-01				

TABLE E.2.—Continued.
(b) Concluded.

TIME 4.50000E+00 SEC		AREA 0.00000E+00 SQ CM		AXIAL POSITION 0.00000E+00 CM			
FLOW PROPERTIES				INTEGRATION INDICATORS			
PRESSURE (ATM) 1.00000		STEPS FROM LAST PRINT 14					
VELOCITY (CM/SEC) 0.00		AVERAGE STEP SIZE 0.14637E+00					
DENSITY (G/CM**3) 4.06227E-05		METHOD ORDER 5					
TEMPERATURE (DEG K) 300.00		TOTAL NUMBER OF STEPS 154					
MASS FLOW RATE (G/SEC) 0.00000E+00		FUNCT EVALUATIONS 166					
ENTROPY (CAL/G/DEG K) 29.9516		JACOBIAN EVALUATIONS 20					
MACH NUMBER 0.0000							
GAMMA 1.6596							
ENTHALPY (CAL/G) 1.50000E+03							
SP. HEAT (CP) (CAL/G/DEG K) 5.00000E+00							
CHEMICAL PROPERTIES							
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
DUMA	2.04359E-05	5.03067E-01	-2.25655E-07	1	1.0000E+00	1.23839E+04	1.00000
DUMB	2.02103E-07	4.97512E-03	-1.02183E-12	2	1.0000E+02	1.22472E+04	1.00000
DUMC	1.99846E-05	4.91958E-01	2.25654E-07	3	1.0000E+02	1.22472E+04	1.00000
				4	1.0000E+00	1.21104E+04	1.00000
DERIVATIVES (CGS UNITS): T		0.00000E+00	RHO	0.00000E+00			
MIXTURE MOLECULAR WEIGHT 1.00000		TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC) 0.00000E+00		MASS FRACTION SUM		1.00000000	
COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 3.999996E-02 S UP TO THIS TIME - 3.499999E-01 S							
***** SENSITIVITY CALCULATIONS *****							
TIME = 4.50000E+00							
SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES							
**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS ****							
DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW							
**** NOTE: FOR CONSTANT TEMPERATURE PROBLEMS NORMALIZED SENSITIVITY COEFFICIENTS W.R.T. M(J) AND E(J) ARE THE SAME AS THE NORMALIZED COEFFICIENTS W.R.T. A(J) ****							
REAC NUM	DUMA	DUMB	DUMC				
1	-5.163D-01	5.031D-01	5.229D-01				
2	4.914D-01	-4.975D-01	-4.975D-01				
3	-4.865D-01	-4.975D-01	5.025D-01				
4	4.617D-01	4.919D-01	-4.771D-01				
(LSLNS) END OF THIS CASE							
SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:							
TOTAL NO. OF STEPS -				154			
TOTAL NO. OF DERIVATIVE EVALUATIONS -				166			
TOTAL NO. OF JACOBIAN EVALUATIONS -				20			
TOTAL CPU TIME -				0.350000 S			
WORK REQUIRED BY SENSITIVITY ROUTINE:							
NO. STEPS =				154			
NO. FUNC. EVAL. =				154			
NO. JAC. EVAL. =				154			
TOTAL REAL SPACE USED =				144			
TOTAL INTEGER SPACE USED =				46			
TOTAL CPU TIME (INCLUDING I/O) REQUIRED * 0.840000 S							
(LSLNS) READ DATA FOR NEXT CASE							

TABLE E.2.—Continued.
(c) Case 3

LEHIS SENSITIVITY AND GENERAL KINETICS PROGRAM									
NASA LEWIS RESEARCH CENTER									
ETHANE PYROLYSIS: KRAMER ET AL, APPL MATH MODELLING, V5, P432, 1981. CASE 3									
REACTION NUMBER		REACTION					REACTION RATE VARIABLES		ACTIVATION ENERGY
1		1*CH ₂ H ₆	>	2*CH ₃			1.20000E+12	0.0000	59218.00
2	1*CH ₂ H ₆	+	1*CH ₃	>	1*CH ₂ H ₅	+	1*CH ₄	0.0000	11943.00
3			1*CH ₂ H ₅	>	1*CH ₂ H ₄	+	1*H	0.0000	34974.00
4	1*H	+	1*CH ₂ H ₆	>	1*CH ₂ H ₅	+	1*H ₂	0.0000	8982.00
5			2*H	>	1*H ₂		6.99000E+13	0.0000	0.00
** INITIAL CONDITIONS **									
TIME	0.00000E+00 SEC		AREA	0.00000E+00 SQ CM		AXIAL POSITION	0.00000E+00 CM		
FLOW PROPERTIES					INTEGRATION INDICATORS				
PRESSURE (ATM)		0.45070			STEPS FROM LAST PRINT		0		
VELOCITY (CM/SEC)		0.00			AVERAGE STEP SIZE		0.00000E+00		
DENSITY (G/CM**3)		1.78937E-04			METHOD ORDER		0		
TEMPERATURE (DEG K)		923.00			TOTAL NUMBER OF STEPS		0		
MASS FLOW RATE (G/SEC)		0.00000E+00			FUNCT EVALUATIONS		0		
ENTROPY (CAL/G/DEG K)		2.6117			JACOBIAN EVALUATIONS		0		
MACH NUMBER		0.0000							
GAMMA		1.0762							
ENTHALPY (CAL/G)		-2.27762E+02							
SP. HEAT (CP) (CAL/G/DEG K)		9.33015E-01							
CHEMICAL PROPERTIES									
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE		
CH ₂ H ₆	5.95080E-06	1.00000E+00	-6.79204E-08	1	1.1414E-02	2.12129E+00	1.00000		
CH ₃	0.00000E+00	0.00000E+00	-1.35841E-07	2	1.1905E+06	0.00000E+00	0.00000		
CH ₂ H ₅	0.00000E+00	0.00000E+00	0.00000E+00	3	1.5700E+03	0.00000E+00	0.00000		
CH ₄	0.00000E+00	0.00000E+00	0.00000E+00	4	9.7088E+08	0.00000E+00	0.00000		
CH ₂ H ₄	0.00000E+00	0.00000E+00	0.00000E+00	5	6.9900E+13	0.00000E+00	0.00000		
H	0.00000E+00	0.00000E+00	0.00000E+00						
H ₂	0.00000E+00	0.00000E+00	0.00000E+00						
DERIVATIVES (CGS UNITS): T		0.00000E+00		RHO	0.00000E+00				
MIXTURE MOLECULAR HEIGHT		30.06940	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)		1.90244E+05	MASS FRACTION SUM	1.00000000		
CPU TIME FOR INITIALIZATION OF LSENS = 0.730000 S									
TIME	2.00000E+01 SEC		AREA	0.00000E+00 SQ CM		AXIAL POSITION	0.00000E+00 CM		
FLOW PROPERTIES					INTEGRATION INDICATORS				
PRESSURE (ATM)		0.69709			STEPS FROM LAST PRINT		31		
VELOCITY (CM/SEC)		0.00			AVERAGE STEP SIZE		0.62654E+00		
DENSITY (G/CM**3)		1.78937E-04			METHOD ORDER		5		
TEMPERATURE (DEG K)		923.00			TOTAL NUMBER OF STEPS		93		
MASS FLOW RATE (G/SEC)		0.00000E+00			FUNCT EVALUATIONS		134		
ENTROPY (CAL/G/DEG K)		3.3191			JACOBIAN EVALUATIONS		20		
MACH NUMBER		0.0000							
GAMMA		1.1225							
ENTHALPY (CAL/G)		3.18711E+02							
SP. HEAT (CP) (CAL/G/DEG K)		9.36808E-01							
CHEMICAL PROPERTIES									
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE		
CH ₂ H ₆	1.91006E-06	2.07526E-01	-9.81539E-08	1	1.1414E-02	6.80881E-01	1.00000		
CH ₃	1.91739E-08	2.08322E-03	-1.46091E-15	2	1.1905E+06	1.36176E+00	1.00000		
CH ₂ H ₅	4.86333E-11	5.28396E-06	-2.53404E-12	3	1.5700E+03	2.38474E+00	1.00000		
CH ₄	1.57517E-06	1.71141E-01	4.36015E-08	4	9.7088E+08	1.02290E+00	1.00000		
CH ₂ H ₄	3.24352E-06	3.52406E-01	7.63556E-08	5	6.9900E+13	6.80945E-01	1.00000		
H	1.76611E-11	1.91886E-06	-1.57847E-12						
H ₂	2.45595E-06	2.66837E-01	5.45544E-08						
DERIVATIVES (CGS UNITS): T		0.00000E+00		RHO	0.00000E+00				
MIXTURE MOLECULAR HEIGHT		19.44135	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)		6.68713E+04	MASS FRACTION SUM	0.99999982		

TABLE E.2.—Continued.
(c) Concluded.

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***** SENSITIVITY CALCULATIONS *****
TIME = 2.00000D+01
SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

**** SENSITIVITY TO INITIAL CONDITIONS ****
DZ(I)/DYZERO(J)*F(J)/Z(I), WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
F(J)= YZERO(J) FOR YZERO(J) NOT EQUAL TO 0
      = 1.0E-4/(INITIAL MWT) FOR YZERO(J) = 0

PARAMETER   C2H6      CH3      C2H5      CH4      C2H4      H      H2
C2H6        7.919D-01 -5.490D-08  9.617D-01  9.104D-01  1.147D+00  5.959D-01  1.223D+00
TEMP        -2.849D+01  2.577D+01 -2.620D+01  1.987D+01  1.167D+01  1.900D+00  9.311D+00

**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS ****
DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
**** NOTE: FOR CONSTANT TEMPERATURE PROBLEMS NORMALIZED SENSITIVITY COEFFICIENTS W.R.T. A(J) AND E(J) ARE
          THE SAME AS THE NORMALIZED COEFFICIENTS W.R.T. A(J) ****

REAC NUM    C2H6      CH3      C2H5      CH4      C2H4      H      H2
1           -8.196D-01  1.000D+00 -2.099D-01  6.433D-01  3.235D-01  7.020D-02  2.210D-01
2           -4.718D-03 -1.000D+00 -5.729D-03  6.888D-03  4.061D-03 -1.359D-03  3.155D-03

(LSENS)      END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:
TOTAL NO. OF STEPS = 93
TOTAL NO. OF DERIVATIVE EVALUATIONS = 134
TOTAL NO. OF JACOBIAN EVALUATIONS = 20
TOTAL CPU TIME = 0.510000 S

WORK REQUIRED BY SENSITIVITY ROUTINE:
NO. STEPS = 93
NO. FUNC. EVAL. = 93
NO. JAC. EVAL. = 93
TOTAL REAL SPACE USED = 424
TOTAL INTEGER SPACE USED = 56

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 1.400000 S

(LSENS)      READ DATA FOR NEXT CASE

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TABLE E.2.—Continued.
(d) Case 4

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM						NASA LEWIS RESEARCH CENTER	
CH4-O2-AR SHOCK IGNITION: BONI & PENNER, COMB SCI & TECH, V15, P99, 1977. CASE 4							
REACTION NUMBER	REACTION				REACTION RATE VARIABLES		ACTIVATION ENERGY
					A	H	
1	M	+ 1*CH4	> 1*CH3	+ 1*H	4.53700E+07	0.0000	0.00
2	1*H	+ 1*CH3	> 1*CH4	+ M	1.10600E+17	0.0000	0.00
3	1*OH	+ 1*CH4	> 1*CH3	+ 1*H2O	2.59000E+13	0.0000	0.00
4	1*CH3	+ 1*H2O	> 1*OH	+ 1*CH4	1.04800E+11	0.0000	0.00
5	1*H	+ 1*CH4	> 1*CH3	+ 1*H2	1.98800E+13	0.0000	0.00
6	1*CH3	+ 1*H2	> 1*H	+ 1*CH4	8.07100E+11	0.0000	0.00
7	1*O	+ 1*CH4	> 1*CH3	+ 1*OH	2.16800E+12	0.0000	0.00
8	1*CH3	+ 1*OH	> 1*O	+ 1*CH4	6.62500E+10	0.0000	0.00
9	1*CH3	+ 1*O	> 1*CH2O	+ 1*H	1.00000E+14	0.0000	0.00
10	1*CH2O	+ 1*H	> 1*CH3	+ 1*O	5.30000E+07	0.0000	0.00
11	1*CH3	+ 1*O2	> 1*CH2O	+ 1*OH	2.00000E+10	0.0000	0.00
12	1*CH2O	+ 1*OH	> 1*CH3	+ 1*O2	4.33700E+04	0.0000	0.00
13	1*CH2O	+ 1*O	> 1*HCO	+ 1*OH	1.58400E+13	0.0000	0.00
14	1*HCO	+ 1*OH	> 1*CH2O	+ 1*O	9.03500E+09	0.0000	0.00
15	1*CH2O	+ 1*OH	> 1*HCO	+ 1*H2O	1.10800E+14	0.0000	0.00
16	1*HCO	+ 1*H2O	> 1*CH2O	+ 1*OH	8.55300E+09	0.0000	0.00
17	1*CH2O	+ 1*H	> 1*HCO	+ 1*H2	5.24000E+12	0.0000	0.00
18	1*HCO	+ 1*H2	> 1*CH2O	+ 1*H	4.21600E+09	0.0000	0.00
19	M	+ 1*CH2O	> 1*HCO	+ 1*H	3.84300E+08	0.0000	0.00
20	1*HCO	+ 1*H	> 1*CH2O	+ M	1.95900E+16	0.0000	0.00
21	1*HCO	+ 1*O	> 1*CO	+ 1*OH	1.00000E+14	0.0000	0.00
22	1*CO	+ 1*OH	> 1*HCO	+ 1*O	1.14400E+05	0.0000	0.00
23	1*HCO	+ 1*OH	> 1*CO	+ 1*H2O	1.00000E+14	0.0000	0.00
24	1*CO	+ 1*H2O	> 1*HCO	+ 1*OH	1.26500E+04	0.0000	0.00
25	1*HCO	+ 1*H	> 1*CO	+ 1*H2	2.00000E+14	0.0000	0.00
26	1*CO	+ 1*H2	> 1*HCO	+ 1*H	2.77100E+05	0.0000	0.00
27	M	+ 1*HCO	> 1*H	+ 1*CO	4.21600E+10	0.0000	0.00
28	1*H	+ 1*CO	> 1*HCO	+ M	3.62800E+12	0.0000	0.00
29	1*CO	+ 1*OH	> 1*CO2	+ 1*H	5.36000E+11	0.0000	0.00
30	1*CO2	+ 1*H	> 1*CO	+ 1*OH	2.28900E+11	0.0000	0.00
31	1*H2	+ 1*OH	> 1*H2O	+ 1*H	1.80700E+13	0.0000	0.00
32	1*H2O	+ 1*H	> 1*H2	+ 1*OH	1.80700E+12	0.0000	0.00
33	1*O	+ 1*H2	> 1*OH	+ 1*H	7.22800E+12	0.0000	0.00
34	1*OH	+ 1*H	> 1*O	+ 1*H2	6.62500E+12	0.0000	0.00
35	1*H	+ 1*O2	> 1*OH	+ 1*O	3.21600E+12	0.0000	0.00
36	1*OH	+ 1*O	> 1*H	+ 1*O2	1.38500E+13	0.0000	0.00
37	1*H	+ 1*OH	> 1*H2O	+ M	2.10400E+15	0.0000	0.00
38	M	+ 1*H2O	> 1*H	+ 1*OH	3.09600E+05	0.0000	0.00
39	1*H	+ 1*H2O	> 2*OH		1.55400E+14	0.0000	0.00
40		2*OH	> 1*H	+ 1*H2O	6.02300E+08	0.0000	0.00
41	1*H	+ 1*O2	> 1*H2	+ M	1.93000E+15	0.0000	0.00
42	M	+ 1*H2O	> 1*H	+ 1*O2	2.16800E+10	0.0000	0.00
43		2*OH	> 1*O	+ 1*H2O	9.45600E+12	0.0000	0.00
44	1*O	+ 1*H2O	> 2*OH		1.20500E+12	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2O , 37) = 16.70000 M(H2O , 38) = 16.70000

TABLE E.2.—Continued.
(d) Continued.

** INITIAL CONDITIONS **									
TIME	0.00000E+00	SEC	AREA	0.00000E+00	SQ CM	AXIAL POSITION	0.00000E+00	CM	
FLOW PROPERTIES					INTEGRATION INDICATORS				
PRESSURE	6.72900				STEPS FROM LAST PRINT	0			
VELOCITY (CM/SEC)	0.00				AVERAGE STEP SIZE	0.00000E+00			
DENSITY (G/CM**3)	1.48828E-03				METHOD ORDER	0			
TEMPERATURE (DEG K)	2000.00								
MASS FLOW RATE (G/SEC)	0.00000E+00				TOTAL NUMBER OF STEPS	0			
ENTROPY (CAL/G/DEG K)	1.3750				FUNCT EVALUATIONS	0			
MACH NUMBER	0.0000				JACOBIAN EVALUATIONS	0			
GAMMA	1.3655								
ENTHALPY (CAL/G)	2.71187E+02								
SP. HEAT (CP) (CAL/G/DEG K)	2.04545E-01								
CHEMICAL PROPERTIES									
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POSI- TIVE DIR RATE		
CH4	5.76075E-06	9.17200E-02	-6.68765E-03	1	4.3370E+07	3.01931E+03	1.00000		
CH3	0.00000E+00	0.00000E+00	6.68765E-03	2	1.1060E+17	0.00000E+00	0.00000		
H	0.00000E+00	0.00000E+00	6.68765E-03	3	2.5900E+13	0.00000E+00	0.00000		
OH	0.00000E+00	0.00000E+00	0.00000E+00	4	1.0480E+11	0.00000E+00	0.00000		
H2O	0.00000E+00	0.00000E+00	0.00000E+00	5	1.9880E+13	0.00000E+00	0.00000		
H2	1.66035E-24	4.04940E-20	0.00000E+00	6	8.0710E+11	0.00000E+00	0.00000		
O	0.00000E+00	0.00000E+00	0.00000E+00	7	2.1680E+12	0.00000E+00	0.00000		
CH2O	0.00000E+00	0.00000E+00	0.00000E+00	8	6.6250E+10	0.00000E+00	0.00000		
O2	7.52150E-06	1.83440E-01	0.00000E+00	9	1.0000E+14	0.00000E+00	0.00000		
HCO	0.00000E+00	0.00000E+00	0.00000E+00	10	5.3000E+07	0.00000E+00	0.00000		
CO	0.00000E+00	0.00000E+00	0.00000E+00	11	2.0000E+10	0.00000E+00	0.00000		
CO2	1.66035E-24	4.04940E-20	0.00000E+00	12	4.3370E+04	0.00000E+00	0.00000		
H02	0.00000E+00	0.00000E+00	0.00000E+00	13	1.5840E+13	0.00000E+00	0.00000		
AR	2.97202E-05	7.24840E-01	0.00000E+00	14	9.0350E+09	0.00000E+00	0.00000		
				15	1.1080E+14	0.00000E+00	0.00000		
				16	8.5530E+09	0.00000E+00	0.00000		
				17	5.2400E+12	0.00000E+00	0.00000		
				18	4.2160E+09	0.00000E+00	0.00000		
				19	3.8430E+08	0.00000E+00	0.00000		
				20	1.9590E+16	0.00000E+00	0.00000		
				21	1.0000E+14	0.00000E+00	0.00000		
				22	1.1440E+05	0.00000E+00	0.00000		
				23	1.0000E+14	0.00000E+00	0.00000		
				24	1.2650E+04	0.00000E+00	0.00000		
				25	2.0000E+14	0.00000E+00	0.00000		
				26	2.7710E+05	0.00000E+00	0.00000		
				27	4.2160E+10	0.00000E+00	0.00000		
				28	3.6280E+12	0.00000E+00	0.00000		
				29	5.3600E+11	0.00000E+00	0.00000		
				30	2.2890E+11	0.00000E+00	0.00000		
				31	1.8070E+13	0.00000E+00	0.00000		
				32	1.8070E+12	0.00000E+00	0.00000		
				33	7.2280E+12	0.00000E+00	0.00000		
				34	6.6250E+12	0.00000E+00	0.00000		
				35	3.2160E+12	0.00000E+00	0.00000		
				36	1.3850E+13	0.00000E+00	0.00000		
				37	2.1040E+15	0.00000E+00	0.00000		
				38	3.0960E+03	0.00000E+00	0.00000		
				39	1.5540E+14	0.00000E+00	0.00000		
				40	6.0230E+08	0.00000E+00	0.00000		
				41	1.9300E+15	0.00000E+00	0.00000		
				42	2.1680E+10	0.00000E+00	0.00000		
				43	9.4560E+12	0.00000E+00	0.00000		
				44	1.2050E+12	0.00000E+00	0.00000		
DERIVATIVES (CGS UNITS): T			0.00000E+00	RHO	0.00000E+00				
MIXTURE MOLECULAR WEIGHT	36.29719		TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)	5.16488E+08	MASS FRACTION SUM	1.00000000			

CPU TIME FOR INITIALIZATION OF LSENS = 0.140000 S

TABLE E.2.—Continued.
(d) Continued.

TIME 2.50000E-05 SEC		AREA 0.00000E+00 SQ CM		AXIAL POSITION 0.00000E+00 CM			
FLOW PROPERTIES				INTEGRATION INDICATORS			
PRESSURE (ATM)	6.83904	STEPS FROM LAST PRINT		92			
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE		0.28285E-06			
DENSITY (G/CM**3)	1.48828E-03	METHOD ORDER		3			
TEMPERATURE (DEG K)	2000.00	TOTAL NUMBER OF STEPS		92			
MASS FLOW RATE (G/SEC)	0.00000E+00	FUNCT EVALUATIONS		123			
ENTROPY (CAL/G/DEG K)	1.4038	JACOBIAN EVALUATIONS		21			
MACH NUMBER	0.0000						
GAMMA	1.3809						
ENTHALPY (CAL/G)	2.20707E+02						
SP. HEAT (CP) (CAL/G/DEG K)	2.01718E-01						
CHEMICAL PROPERTIES							
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
CH4	2.33149E-06	5.59472E-02	-7.80458E-02	1	4.3370E+07	1.90244E+05	1.00000
CH3	3.51582E-07	8.43670E-03	-9.61705E-03	2	1.1060E+17	2.48077E+03	1.00000
H	3.39090E-09	8.13694E-05	2.25868E-04	3	2.5900E+13	4.79050E+04	1.00000
OH	1.75717E-09	4.21658E-05	1.03282E-04	4	1.0480E+11	2.46003E+04	1.00000
H2O	1.44637E-06	3.47076E-02	1.37114E-01	5	1.9880E+13	7.09575E+04	1.00000
H2	4.82428E-07	1.15765E-02	3.94364E-02	6	8.0710E+11	6.18046E+04	1.00000
O	1.24225E-09	2.98095E-05	8.06246E-05	7	2.1680E+12	2.83488E+03	1.00000
CH2O	3.82100E-07	9.16900E-03	-6.56945E-03	8	6.6250E+10	1.84783E+01	1.00000
O2	6.25565E-06	1.50113E-01	-1.12830E-01	9	1.0000E+14	1.97183E+04	1.00000
HCO	3.41967E-08	8.20597E-04	7.02750E-04	10	5.3000E+07	3.10028E-02	1.00000
CO	6.59063E-07	1.58151E-02	9.29106E-02	11	2.0000E+10	1.98592E+04	1.00000
CO2	2.32046E-09	5.56826E-05	6.18934E-04	12	4.3370E+04	1.31466E-05	1.00000
HO2	1.16503E-09	2.79566E-05	3.96000E-05	13	1.5840E+13	3.39449E+03	1.00000
AR	2.97202E-05	7.13178E-01	0.00000E+00	14	9.0350E+09	2.45110E-01	1.00000
				15	1.1080E+14	3.35865E+04	1.00000
				16	8.5530E+09	1.90992E+02	1.00000
				17	5.2400E+12	3.06519E+03	1.00000
				18	4.2160E+09	3.14016E+01	1.00000
				19	3.8430E+08	2.76271E+03	1.00000
				20	1.9590E+16	4.27388E+01	1.00000
				21	1.0000E+14	1.91791E+03	1.00000
				22	1.1440E+05	5.98138E-05	1.00000
				23	1.0000E+14	2.71289E+03	1.00000
				24	1.2650E+04	5.44414E-03	1.00000
				25	2.0000E+14	1.04704E+04	1.00000
				26	2.7710E+05	3.97768E-02	1.00000
				27	4.2160E+10	2.71252E+04	1.00000
				28	3.6280E+12	1.52545E-01	1.00000
				29	5.3600E+11	2.80246E+02	1.00000
				30	2.2890E+11	8.13147E-01	1.00000
				31	1.8070E+13	6.91575E+03	1.00000
				32	1.8070E+12	4.00116E+03	1.00000
				33	7.2280E+12	1.95566E+03	1.00000
				34	6.6250E+12	1.78217E+01	1.00000
				35	3.2160E+12	3.07991E+04	1.00000
				36	1.3850E+13	1.36492E+01	1.00000
				37	2.1040E+15	5.64390E-01	1.00000
				38	5.0960E+03	1.30158E-01	1.00000
				39	1.5540E+14	2.77165E+02	1.00000
				40	6.0230E+08	8.39606E-04	1.00000
				41	1.9300E+15	7.70253E+02	1.00000
				42	2.1680E+10	4.75210E+02	1.00000
				43	9.4560E+12	1.31817E+01	1.00000
				44	1.2050E+12	9.77482E+02	1.00000
DERIVATIVES (CGS UNITS): T		0.00000E+00	RHO	0.00000E+00			
MIXTURE MOLECULAR WEIGHT		35.71319	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)		-4.13916E+09	MASS FRACTION SUM	1.00000001

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 5.130000E+00 S UP TO THIS TIME - 5.130000E+00 S

TABLE E.2.—Continued.
(d) Concluded.

***** SENSITIVITY CALCULATIONS *****												
TIME = 2.50000D-05												
SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES												
***** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS *****												
DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW												
***** NOTE: FOR CONSTANT TEMPERATURE PROBLEMS NORMALIZED SENSITIVITY COEFFICIENTS W.R.T. R(J) AND E(J) ARE THE SAME AS THE NORMALIZED COEFFICIENTS W.R.T. A(J) *****												
REAC NUM	CH4	CH3	H	OH	H2O	H2	D	CH2O	O2	HCO	CO	
1	-3.319D-01	-1.247D-01	8.069D-01	6.898D-01	8.722D-01	8.049D-01	6.668D-01	-1.152D-01	-1.669D-01	3.045D-01	1.283D+00	
2	3.728D-02	-6.432D-02	-1.712D-01	-1.390D-01	-6.647D-02	-8.629D-02	-1.083D-01	-1.042D-03	1.291D-02	-7.517D-02	-9.244D-02	
3	-5.708D-02	2.276D-01	6.977D-02	-5.303D-01	8.713D-03	-1.111D-01	-1.280D-01	4.872D-01	-4.995D-03	7.549D-02	-2.027D-01	
4	2.381D-02	-1.010D-01	-2.376D-02	2.608D-01	-5.333D-03	4.701D-02	5.876D-02	-1.913D-01	2.114D-03	9.591D-03	7.887D-02	
5	8.496D-02	2.603D-01	-5.873D-01	-3.950D-01	-4.300D-01	5.616D-02	-6.956D-01	1.675D-01	7.324D-02	6.018D-02	-5.296D-01	
6	-4.008D-02	-1.967D-01	4.772D-01	2.912D-01	2.593D-01	-8.890D-02	5.700D-01	-1.167D-01	-4.318D-02	4.350D-02	3.089D-01	
7	-2.685D-02	9.706D-02	4.945D-02	1.261D-01	7.261D-02	-3.955D-02	-1.115D-01	-3.387D-02	-1.071D-02	4.634D-02	5.984D-02	
8	1.063D-04	-5.710D-04	-2.170D-04	-6.599D-04	-2.687D-04	2.526D-04	7.550D-04	2.007D-04	3.500D-05	-2.131D-04	-1.746D-04	
9	3.510D-02	-2.348D-01	-4.920D-02	-3.311D-01	-1.302D-01	1.475D-01	-5.521D-01	2.056D-01	1.517D-02	-4.792D-02	-1.143D-01	
10	-3.299D-08	3.245D-07	4.680D-08	4.470D-07	1.311D-07	-2.015D-07	8.750D-07	-2.910D-07	-1.241D-08	5.746D-08	1.079D-07	
11	-2.627D-01	-4.731D-01	4.115D-01	4.310D-01	7.612D-01	6.661D-01	4.842D-01	1.151D-01	1.507D-01	4.018D-01	1.087D+00	
12	5.889D-11	1.446D-10	-7.731D-11	-1.391D-10	-1.662D-10	-1.391D-10	-1.033D-10	-1.038D-10	3.435D-11	-1.955D-10	-2.139D-10	
13	-9.422D-03	6.505D-02	2.924D-02	1.200D-01	4.350D-02	-1.805D-02	-1.160D-01	-1.182D-01	-4.972D-03	6.078D-02	6.446D-02	
14	4.210D-07	-3.994D-06	-1.560D-06	-7.329D-06	-2.162D-06	1.086D-06	8.489D-06	7.354D-06	2.180D-07	-3.189D-06	-5.428D-06	
15	4.269D-02	-1.945D-01	-2.603D-02	-3.000D-01	1.409D-02	1.867D-01	1.395D-01	5.428D-01	8.691D-04	6.994D-02	2.647D-01	
16	-2.055D-04	9.345D-04	1.264D-04	1.886D-03	-8.884D-06	-8.094D-04	-6.080D-04	2.306D-03	-1.124D-05	-8.719D-05	-1.065D-03	
17	7.992D-03	-2.058D-02	-2.840D-02	-9.167D-03	-1.052D-02	2.631D-02	-8.809D-03	-6.272D-02	2.129D-03	8.556D-03	-1.857D-02	
18	-7.032D-05	1.961D-04	2.862D-04	1.037D-04	8.944D-05	-2.383D-04	1.111D-04	5.578D-04	-1.078D-04	-1.264D-03	-1.294D-03	
19	-8.995D-02	3.298D-02	3.295D-01	2.920D-03	-1.920D-03	-6.806D-04	-1.260D-03	-1.682D-03	7.722D-04	1.282D-04	-1.264D-03	
20	3.567D-04	-6.411D-04	-2.284D-03	-1.920D-03	-1.067D-02	-5.730D-02	-1.182D-01	-1.973D-02	3.425D-03	-6.290D-02	-2.633D-02	
21	9.570D-03	1.365D-02	-6.007D-02	-7.704D-03	-1.067D-02	-5.730D-02	-1.182D-01	-1.973D-02	3.425D-03	-6.290D-02	-2.633D-02	
22	-1.782D-10	-2.795D-10	1.399D-09	4.156D-11	1.352D-10	1.357D-09	-3.227D-09	5.044D-10	-5.124D-11	1.703D-09	3.977D-10	
23	2.141D-02	-3.890D-02	-1.047D-01	-1.183D-01	-3.878D-02	-5.702D-02	-6.428D-02	1.712D-02	7.439D-03	-1.148D-01	5.850D-02	
24	-2.274D-08	5.939D-08	1.379D-07	1.740D-07	3.480D-08	6.156D-08	8.079D-08	-2.376D-08	6.664D-09	1.949D-07	5.196D-08	
25	7.995D-02	-1.585D-01	-4.490D-01	-3.506D-01	-1.454D-01	-1.495D-01	-2.879D-01	4.087D-03	2.744D-02	-4.174D-01	-1.777D-01	
26	-2.041D-07	4.845D-07	1.366D-06	1.032D-06	3.467D-07	3.618D-07	8.906D-07	-1.012D-08	-6.480D-08	1.370D-06	3.954D-07	
27	-1.298D-01	1.794D-01	6.796D-01	5.260D-01	2.485D-01	3.326D-01	5.241D-01	-1.258D-01	7.439D-03	-1.148D-01	5.850D-02	
28	3.263D-07	-8.015D-07	-2.598D-06	-1.909D-06	-4.975D-07	-8.700D-07	-2.094D-06	1.597D-08	9.822D-08	2.442D-06	8.565D-07	
29	-3.552D-04	3.613D-05	5.231D-03	-1.074D-03	-4.015D-04	3.494D-03	4.733D-03	1.235D-03	2.028D-04	-2.633D-04	-3.008D-03	
30	5.927D-07	-2.474D-07	-1.257D-05	3.838D-06	1.132D-06	-6.688D-06	-1.147D-05	-2.748D-06	3.296D-07	1.644D-06	6.285D-06	
31	-8.104D-05	7.692D-05	5.921D-02	-4.415D-02	-2.086D-02	-2.072D-02	-2.802D-02	-1.907D-02	1.737D-03	4.728D-03	-6.772D-04	
32	3.940D-05	-4.533D-05	-3.380D-02	2.608D-02	-9.824D-03	2.138D-02	-2.156D-02	-6.034D-02	-1.959D-02	2.748D-03	1.526D-02	
33	-7.407D-03	3.984D-02	2.860D-02	6.023D-02	-5.427D-04	-1.820D-04	1.965D-04	5.522D-04	1.790D-04	-2.275D-05	-1.463D-04	
34	6.338D-05	-3.640D-04	-2.562D-04	-8.778D-01	6.709D-01	1.693D-01	1.157D+00	-8.570D-02	1.194D-01	5.463D-01	7.946D-01	
35	2.196D-01	-1.163D-02	3.051D-01	-3.234D-04	-1.892D-04	-3.063D-05	-4.715D-04	2.065D-05	3.337D-05	-2.119D-04	-2.143D-04	
36	6.190D-05	-7.743D-06	-8.059D-05	-1.844D-05	-5.111D-06	-8.111D-06	-1.213D-05	1.946D-06	9.838D-07	-8.348D-06	-7.926D-06	
37	3.043D-06	-6.511D-06	8.663D-06	8.522D-06	3.813D-06	4.927D-06	6.029D-06	-9.966D-07	7.350D-07	3.867D-06	5.788D-06	
38	-1.898D-06	2.364D-06	8.663D-06	1.560D-03	8.949D-04	-5.906D-03	-7.056D-03	-2.149D-03	6.936D-05	6.605D-05	7.987D-04	
39	4.957D-04	5.447D-04	-7.330D-03	-5.312D-09	-1.552D-09	2.163D-08	2.407D-08	6.582D-09	4.901D-10	6.584D-10	5.083D-09	
40	-2.175D-09	-2.328D-09	2.502D-08	-1.512D-05	-2.177D-05	-1.222D-02	-1.416D-02	-2.639D-03	4.540D-04	1.597D-03	5.648D-03	
41	1.997D-03	4.164D-04	-1.542D-02	-1.512D-05	-2.177D-05	-1.222D-02	-1.416D-02	-2.639D-03	4.540D-04	1.597D-03	5.648D-03	
42	-1.364D-03	-4.455D-04	9.951D-03	1.083D-03	1.601D-03	8.197D-03	9.182D-03	1.694D-03	-3.387D-04	1.112D-03	4.004D-03	
43	3.958D-05	-2.732D-04	-9.129D-05	-5.145D-04	-1.202D-04	1.147D-04	5.004D-04	2.116D-04	1.371D-03	-1.265D-04	-1.088D-04	
44	-2.420D-03	1.839D-02	5.592D-03	3.570D-02	7.314D-03	-7.596D-03	-3.700D-02	-1.445D-02	-7.868D-04	8.903D-03	6.567D-03	
REAC NUM	CO2	HO2										
1	2.403D+00	4.339D-01										
2	-1.772D-01	-9.777D-02										
3	-9.206D-01	-2.923D-02										
4	3.340D-01	-8.113D-03	(LENS) END OF THIS CASE									
5	-1.062D+00	-3.508D-01										
6	6.225D-01	2.916D-01										
7	1.697D-01	2.248D-02										
8	-6.472D-04	-9.945D-05										
9	-3.751D-01	-1.632D-02										
10	4.001D-07	1.349D-08										
11	1.858D+00	1.671D-01										
12	-3.396D-10	-2.540D-11										
13	1.626D-01	7.981D-10										
14	-8.218D-06	-7.706D-07										
15	9.606D-02	-3.899D-03										
16	2.931D-04	1.435D-05										
17	1.585D-02	-1.568D-02										
18	-1.097D-04	1.558D-04										
19	6.817D-01	1.905D-01										
20	-2.211D-03	-1.302D-03										
21	-2.803D-02	-3.582D-02										
22	3.268D-10	7.981D-10										
23	-1.325D-07	-5.979D-02										
24	1.522D-07	7.453D-08										
25	-3.599D-01	-2.562D-01										
26	8.419D-07	7.432D-07										
27	7.300D-01	3.909D-01										
28	-1.484D-06	-1.383D-06										
29	9.971D-01	2.895D-03										
30	-1.915D-03	-6.486D-06										
31	-2.878D-02	3.546D-02										
32	1.755D-02	-1.903D-02										
33	5.220D-02	1.472D-02										
34	-4.462D-04	-1.331D-04										
35	1.593D+00	1.065D-01	(LENS) READ DATA FOR NEXT CASE									
36	-4.344D-04	-2.501D-05										
37	-1.726D-05	-9.929D-06										
38	1.192D-05	4.871D-06										
39	1.068D-05	-3.502D-03										
40	8.026D-10	1.056D-06										
41	-7.250D-03	9.904D-01										
42	5.261D-03	-6.182D-01										
43	-4.557D-04	-4.132D-05										
44	2.877D-02	2.483D-03										
SUMMARY OF COMPUTATION/WORK REQUIRED FOR PROBLEM:												
TOTAL NO. OF STEPS = 92												
TOTAL NO. OF DERIVATIVE EVALUATIONS = 123												
TOTAL NO. OF JACOBIAN EVALUATIONS = 21												
TOTAL CPU TIME = 5.130000 S												
WORK REQUIRED BY SENSITIVITY ROUTINE:												
NO. STEPS = 92												
NO. FUNC. EVAL. = 92												
NO. JAC. EVAL. = 92												
TOTAL REAL SPACE USED = 3924												
TOTAL INTEGER SPACE USED = 66												
TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 6.800000 S												

TABLE E.2.—Continued.
(e) Case 5

LEHIS SENSITIVITY AND GENERAL KINETICS PROGRAM

NASA LEHIS RESEARCH CENTER

FORMALDEHYDE OXID.: DOUGHERTY ET AL, J. CHEM PHYS, V71, P1794, 1979.

CASE 5

REACTION NUMBER	REACTION						REACTION RATE VARIABLES A	N	ACTIVATION ENERGY	
1	1*HCO	+	1*O2	>	1*CO	+	1*H2O2	6.02000E+10	0.0000	0.00
2	1*H2O2	+	1*CH2O	>	1*H2O2	+	1*HCO	3.43000E+10	0.0000	0.00
3	M	+	1*H2O2	>	2*OH			4.01000E+06	0.0000	0.00
4	1*CH2O	+	1*OH	>	1*HCO	+	1*H2O	9.64000E+13	0.0000	0.00
5	1*OH	+	1*H2O2	>	1*H2O	+	1*H2O2	3.07000E+12	0.0000	0.00
6			1*H2O2	>	1*H2O2H			1.05000E+02	0.0000	0.00
7			1*H2O2	>	1*H2O2H			1.05000E+01	0.0000	0.00
8			2*H2O2	>	1*H2O2	+	1*O2	1.81000E+12	0.0000	0.00
9	1*CO	+	1*OH	>	1*CO2	+	1*H	1.99000E+11	0.0000	0.00
10	1*CO	+	1*H2O2	>	1*CO2	+	1*OH	7.23000E+08	0.0000	0.00
11	1*CH2O	+	1*H	>	1*HCO	+	1*H2	1.63000E+12	0.0000	0.00
12	1*H	+	1*O2	>	1*OH	+	1*O	3.32000E+10	0.0000	0.00
13	1*H	+	1*O2	>	1*H2O	+	M	3.63000E+15	0.0000	0.00
14	M	+	1*H2O2	>	1*H	+	1*O2	2.83000E+05	0.0000	0.00
15	1*O	+	1*H2	>	1*OH	+	1*H	1.82000E+11	0.0000	0.00
16	1*CH2O	+	1*O	>	1*HCO	+	1*OH	6.02000E+13	0.0000	0.00
17	1*H	+	1*H2O2	>	1*H2O	+	1*H2	7.83000E+11	0.0000	0.00
18	1*H	+	1*H2O2	>	1*H2O	+	1*OH	3.55000E+12	0.0000	0.00
19	1*O	+	1*H2O2	>	1*OH	+	1*H2O2	6.02000E+10	0.0000	0.00
20			1*HCO	>	1*H	+	1*CO	4.60000E-12	0.0000	0.00
21	1*H2	+	1*OH	>	1*H2O	+	1*H	6.02000E+12	0.0000	0.00
22	1*CH2O	+	1*O2	>	1*HCO	+	1*H2O2	1.75000E+04	0.0000	0.00
23	1*H	+	1*H2O2	>	2*OH			3.01000E+12	0.0000	0.00
24	1*H2O2	+	1*H	>	1*H2O	+	1*O	3.01000E+13	0.0000	0.00
25	1*H	+	1*H2O2	>	1*H2	+	1*O2	2.71000E+13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0

** INITIAL CONDITIONS **

TIME 0.00000E+00 SEC AREA 0.00000E+00 SQ CM AXIAL POSITION 0.00000E+00 CM

FLOW PROPERTIES

PRESSURE 0.91807
(ATM)
VELOCITY 0.00
(CM/SEC)
DENSITY 3.37842E-04
(G/CM**3)
TEMPERATURE 952.00
(DEG K)
MASS FLOW RATE 0.00000E+00
(G/SEC)
ENTROPY 2.0112
(CAL/G/DEG K)
MACH NUMBER 0.0000
GAMMA 1.3330
ENTHALPY -2.07869E+02
(CAL/G)
SP. HEAT (CP) 2.7673/E-01
(CAL/G/DEG K)

INTEGRATION INDICATORS

STEPS FROM LAST PRINT 0
AVERAGE STEP SIZE 0.00000E+00
METHOD ORDER 0
TOTAL NUMBER OF STEPS 0
FUNCT EVALUATIONS 0
JACOBIAN EVALUATIONS 0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSTI- TIVE DIR RATE
HCO	0.00000E+00	0.00000E+00	4.14841E-09	1	6.0200E+10	0.00000E+00	0.00000
O2	2.10900E-06	1.79453E-01	-4.14841E-09	2	3.4300E+10	0.00000E+00	0.00000
CO	4.69900E-06	3.99832E-01	0.00000E+00	3	4.0100E+06	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	4.14841E-09	4	9.6400E+13	0.00000E+00	0.00000
CH2O	1.12400E-07	9.56400E-03	-4.14841E-09	5	3.0700E+12	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	6	1.0500E+02	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	0.00000E+00	7	1.0500E+01	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	8	1.8100E+12	0.00000E+00	0.00000
H2O2H	0.00000E+00	0.00000E+00	0.00000E+00	9	1.9900E+11	0.00000E+00	0.00000
H2O2H	0.00000E+00	0.00000E+00	0.00000E+00	10	7.2300E+08	0.00000E+00	0.00000
CO2	0.00000E+00	0.00000E+00	0.00000E+00	11	1.6300E+12	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	0.00000E+00	12	3.3200E+10	0.00000E+00	0.00000
H2	0.00000E+00	0.00000E+00	0.00000E+00	13	3.6300E+15	0.00000E+00	0.00000
O	0.00000E+00	0.00000E+00	0.00000E+00	14	2.8300E+05	0.00000E+00	0.00000
H2	4.83200E-06	4.11150E-01	0.00000E+00	15	1.8200E+11	0.00000E+00	0.00000
				16	6.0200E+13	0.00000E+00	0.00000
				17	7.8300E+11	0.00000E+00	0.00000
				18	3.5500E+12	0.00000E+00	0.00000
				19	6.0200E+10	0.00000E+00	0.00000
				20	4.6000E-12	0.00000E+00	0.00000
				21	6.0200E+12	0.00000E+00	0.00000
				22	1.7500E+04	3.6345E-02	1.00000
				23	3.0100E+12	0.00000E+00	0.00000
				24	3.0100E+13	0.00000E+00	0.00000
				25	2.7100E+13	0.00000E+00	0.00000

TABLE E.2.—Continued.
(c) Continued.

DERIVATIVES (CGS UNITS): T		0.00000E+00	RHO	0.00000E+00			
MIXTURE MOLECULAR WEIGHT	28.74664	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)		1.40297E+03	MASS FRACTION SUM	1.00000000	
CPU TIME FOR INITIALIZATION OF LSENS =				1.040001 S			
TIME	5.00000E-03 SEC	AREA	0.00000E+00 SQ CM	AXIAL POSITION	0.00000E+00 CM		
FLOW PROPERTIES				INTEGRATION INDICATORS			
PRESSURE (ATM)	0.91807	STEPS FROM LAST PRINT		10			
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE		0.51495E-03			
DENSITY (G/CM**3)	3.37842E-04	METHOD ORDER		3			
TEMPERATURE (DEG K)	952.00	TOTAL NUMBER OF STEPS		15			
MASS FLOW RATE (G/SEC)	0.00000E+00	FUNCT EVALUATIONS		15			
ENTROPY (CAL/G/DEG K)	2.0113	JACOBIAN EVALUATIONS		4			
MACH NUMBER	0.0000						
GAMMA	1.3330						
ENTHALPY (CAL/G)	-2.08171E+02						
SP. HEAT (CP) (CAL/G/DEG K)	2.76736E-01						
CHEMICAL PROPERTIES							
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE
HCO	5.99396E-12	5.10019E-07	2.49009E-09	1	6.0200E+10	6.66295E+00	1.00000
O2	2.10758E-06	1.79331E-01	-7.61730E-07	2	3.4300E+10	3.23812E+00	1.00000
CO	4.69973E-06	3.99895E-01	3.98642E-07	3	4.0100E+06	2.38579E-01	1.00000
HO2	9.70807E-11	8.26048E-06	3.75318E-08	4	9.6400E+13	5.20526E+00	1.00000
CH2O	1.10992E-07	9.44422E-03	-7.62981E-07	5	3.0700E+12	5.31397E-04	1.00000
H2O2	5.77813E-10	4.91654E-05	2.98456E-07	6	1.0500E+02	5.31556E-01	1.00000
OH	3.41917E-14	2.90933E-09	-1.01196E-10	7	1.0500E+01	8.93089E-03	1.00000
H2O	6.57434E-10	5.59403E-05	3.66366E-07	8	1.8100E+12	1.49457E-01	1.00000
H2O2H	8.91753E-11	7.58782E-06	6.06704E-08	9	1.9900E+11	2.80168E-01	1.00000
H2O2H	1.88581E-12	1.60461E-07	1.01935E-09	10	7.2300E+08	2.89013E+00	1.00000
CO2	6.67303E-10	5.67800E-05	3.61849E-07	11	1.6300E+12	1.46432E-01	1.00000
H	9.25807E-14	7.86056E-09	5.21113E-11	12	3.3200E+10	5.66337E-02	1.00000
H2	5.05162E-11	2.59659E-06	1.69919E-08	13	5.6300E+15	7.27731E-02	1.00000
O	1.00921E-15	8.58722E-11	-9.34028E-12	14	2.8300E+05	2.82891E-03	1.00000
N2	4.83200E-06	4.11149E-01	0.00000E+00	15	1.8200E+11	4.91082E-08	1.00000
				16	6.0200E+13	5.90803E-02	1.00000
				17	7.8300E+11	3.66187E-04	1.00000
				18	3.5500E+12	1.66023E-03	1.00000
				19	6.0200E+10	3.07565E-07	1.00000
				20	4.6000E-12	2.41571E-16	1.00000
				21	6.0200E+12	5.50326E-05	1.00000
				22	1.7500E+04	5.58664E-02	1.00000
				23	3.0100E+12	2.36512E-04	1.00000
				24	3.0100E+13	2.36512E-03	1.00000
				25	2.7100E+13	2.12939E-03	1.00000
DERIVATIVES (CGS UNITS): T		0.00000E+00	RHO	0.00300E+00			
MIXTURE MOLECULAR WEIGHT	28.74658	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)		-4.92865E+05	MASS FRACTION SUM	1.00000000	

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 3.199997E-01 S UP TO THIS TIME - 4.099989E-01 S

TABLE E.2.—Continued.
(c) Continued.

***** SENSITIVITY CALCULATIONS *****											
TIME = 5.00000D-03											
SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES											
***** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS *****											
DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW											
***** NOTE: FOR CONSTANT TEMPERATURE PROBLEMS NORMALIZED SENSITIVITY COEFFICIENTS W.R.T. H(J) AND E(J) ARE THE SAME AS THE NORMALIZED COEFFICIENTS H.R.T. A(J) *****											
REAC NUM	HCO	O2	CO	HO2	CH2O	H2O2	OH	H2O	H2O2H	HO2H	CO2
1	-9.231D-01	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
2	1.236D+00	0.000D+00	0.000D+00	7.054D-01	0.000D+00	1.493D+00	8.297D-01	5.878D-01	1.358D+00	4.858D-01	4.952D-01
3	7.700D-01	0.000D+00	0.000D+00	7.224D-01	0.000D+00	4.922D-01	8.383D-01	6.084D-01	3.565D-01	5.095D-01	5.183D-01
4	-2.137D-01	0.000D+00	0.000D+00	-2.124D-01	0.000D+00	-1.836D-01	-1.162D+00	-1.233D-01	-1.512D-01	-1.736D-01	-2.548D-01
5	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
6	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	-1.827D-01	0.000D+00	0.000D+00	8.576D-01	0.000D+00	0.000D+00
7	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	9.833D-01	0.000D+00
8	-3.056D-01	0.000D+00	0.000D+00	-3.195D-01	0.000D+00	-1.770D-01	-3.016D-01	-1.780D-01	-1.130D-01	-1.862D-01	-1.856D-01
9	2.142D-01	0.000D+00	0.000D+00	2.128D-01	0.000D+00	1.841D-01	1.624D-01	1.238D-01	1.517D-01	1.740D-01	2.552D-01
10	5.976D-01	0.000D+00	0.000D+00	1.662D-01	0.000D+00	1.377D-01	1.027D+00	1.013D+00	1.108D-01	1.325D-01	1.122D+00
11	-1.235D-01	0.000D+00	0.000D+00	-1.227D-01	0.000D+00	-1.065D-01	-1.397D-01	-1.178D-01	0.000D+00	-1.007D-01	-1.022D-01
12	2.034D-01	0.000D+00	0.000D+00	1.915D-01	0.000D+00	1.648D-01	2.164D-01	1.798D-01	1.352D-01	1.554D-01	1.576D-01
13	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
14	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
15	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
16	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
17	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
18	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
19	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
20	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
21	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
22	6.836D-01	0.000D+00	0.000D+00	6.756D-01	0.000D+00	8.101D-01	7.048D-01	8.183D-01	8.805D-01	8.094D-01	8.106D-01
23	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
24	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
25	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00

REAC NUM	H	H2	O
1	0.000D+00	0.000D+00	0.000D+00
2	8.133D-01	5.845D-01	8.527D-01
3	8.255D-01	6.063D-01	8.599D-01
4	-1.149D+00	-1.112D+00	-1.158D+00
5	0.000D+00	0.000D+00	0.000D+00
6	0.000D+00	0.000D+00	0.000D+00
7	0.000D+00	0.000D+00	0.000D+00
8	-2.962D-01	-1.775D-01	-3.109D-01
9	1.150D+00	1.112D+00	1.159D+00
10	1.019D+00	1.005D+00	1.031D+00
11	-6.550D-01	3.487D-01	-6.602D-01
12	0.000D+00	0.000D+00	9.810D-01
13	-3.246D-01	-3.156D-01	-3.273D-01
14	0.000D+00	0.000D+00	0.000D+00
15	0.000D+00	0.000D+00	0.000D+00
16	0.000D+00	0.000D+00	-9.999D-01
17	0.000D+00	0.000D+00	0.000D+00
18	0.000D+00	0.000D+00	0.000D+00
19	0.000D+00	0.000D+00	0.000D+00
20	0.000D+00	0.000D+00	0.000D+00
21	0.000D+00	0.000D+00	0.000D+00
22	6.940D-01	8.176D-01	7.297D-01
23	0.000D+00	0.000D+00	0.000D+00
24	0.000D+00	0.000D+00	0.000D+00
25	0.000D+00	0.000D+00	0.000D+00

TABLE E.2.—Continued.
(c) Concluded.

TIME = 5.00000E-03

*** REACTION IMPORTANCE FOR NORMALIZED SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF Y(1) WRT PREEXPONENTIAL CONSTANTS ***

VARIABLE	REACTION NUMBER									
	NORMALIZED SENSITIVITY COEFFICIENT									
	2	1	3	22	10	8	9	4	12	11
HCO	1.236E+00	-9.231E-01	7.700E-01	6.836E-01	5.976E-01	-3.056E-01	2.142E-01	-2.137E-01	2.034E-01	-1.235E-01
O2										
CO										
	3	2	22	8	9	4	12	10	11	
H02	7.224E-01	7.054E-01	6.756E-01	-3.195E-01	2.128E-01	-2.124E-01	1.915E-01	1.662E-01	-1.227E-01	
CH2O										
	2	22	3	9	4	6	8	12	10	11
H2O2	1.493E+00	8.101E-01	4.922E-01	1.841E-01	-1.836E-01	-1.827E-01	-1.770E-01	1.648E-01	1.377E-01	-1.065E-01
OH	4	10	3	2	22	8	12	9	11	
	-1.162E+00	1.027E+00	8.583E-01	8.297E-01	7.048E-01	-3.016E-01	2.164E-01	1.624E-01	-1.397E-01	
H2O	10	22	3	2	12	8	9	4	11	
	1.013E+00	8.183E-01	6.084E-01	5.878E-01	1.798E-01	-1.780E-01	1.238E-01	-1.233E-01	-1.178E-01	
H2O2H	2	22	6	3	9	4	12	8	10	
	1.358E+00	8.805E-01	8.576E-01	3.565E-01	1.517E-01	-1.112E-01	1.352E-01	-1.130E-01	1.108E-01	
H02H	7	22	3	2	8	9	4	12	10	11
	9.833E-01	8.094E-01	5.095E-01	4.858E-01	-1.862E-01	1.740E-01	-1.736E-01	1.554E-01	1.525E-01	-1.007E-01
CO2	10	22	3	2	9	4	8	12	11	
	1.122E+00	8.106E-01	5.183E-01	4.952E-01	2.552E-01	-2.548E-01	-1.856E-01	1.576E-01	-1.022E-01	
H	9	4	10	3	2	22	11	13	8	
	1.150E+00	-1.149E+00	1.019E+00	8.255E-01	8.133E-01	6.440E-01	-6.550E-01	-3.246E-01	-2.962E-01	
H2	9	4	10	22	3	2	11	13	8	
	1.112E+00	-1.112E+00	1.005E+00	8.176E-01	6.063E-01	5.045E-01	3.487E-01	-3.156E-01	-1.775E-01	
O	9	4	10	16	12	3	2	22	11	13
	1.159E+00	-1.158E+00	1.031E+00	-9.999E-01	9.810E-01	8.599E-01	8.527E-01	7.297E-01	-6.602E-01	-3.275E-01
	8									
	-3.109E-01									

(LSSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS = 13
 TOTAL NO. OF DERIVATIVE EVALUATIONS = 15
 TOTAL NO. OF JACOBIAN EVALUATIONS = 4
 TOTAL CPU TIME = 0.409999 S

WORK REQUIRED BY SENSITIVITY ROUTINE:

NO. STEPS = 13
 NO. FUNC. EVAL. = 13
 NO. JAC. EVAL. = 13
 TOTAL REAL SPACE USED = 2656
 TOTAL INTEGER SPACE USED = 68

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 2.030000 S

(LSSENS) READ DATA FOR NEXT CASE

TABLE E.2.—Continued.
(f) Case 6

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM										NASA LEWIS RESEARCH CENTER	
WET CO OXIDATION: YETTER ET AL, COMB & FLAME, V59, P107, 1985.										CASE 6	
REACTION NUMBER	REACTION					REACTION RATE		VARIABLES		ACTIVATION ENERGY	
						A	N				
1	1*HCO	+	1*H	>	1*CO	+	1*H2	2.00000E+14	0.0000	0.00	
2	1*CO	+	1*H2	>	1*HCO	+	1*H	1.71600E-03	0.0000	0.00	
3	1*HCO	+	1*OH	>	1*CO	+	1*H2O	1.00000E+14	0.0000	0.00	
4	1*CO	+	1*H2O	>	1*HCO	+	1*OH	3.65600E-06	0.0000	0.00	
5	1*HCO	+	1*O	>	1*CO	+	1*OH	3.01200E+13	0.0000	0.00	
6	1*CO	+	1*OH	>	1*O	+	1*HCO	2.86700E-04	0.0000	0.00	
7	1*HCO	+	1*O2	>	1*CO	+	1*H2O2	3.01500E+12	0.0000	0.00	
8	1*CO	+	1*H2O2	>	1*HCO	+	1*O2	2.59000E+06	0.0000	0.00	
9	1*CO	+	1*H2O2	>	1*CO2	+	1*OH	3.08400E+09	0.0000	0.00	
10	1*CO2	+	1*OH	>	1*CO	+	1*H2O	1.77700E-02	0.0000	0.00	
11	1*CO	+	1*OH	>	1*CO2	+	1*H	1.92100E+11	0.0000	0.00	
12	1*CO2	+	1*H	>	1*CO	+	1*OH	7.89000E+08	0.0000	0.00	
13	1*CO2	+	1*O	>	1*CO	+	1*O2	4.43400E+02	0.0000	0.00	
14	1*CO	+	1*O2	>	1*CO2	+	1*O	8.49200E+02	0.0000	0.00	
15	1*H	+	1*O2	>	1*OH	+	1*O	1.12600E+11	0.0000	0.00	
16	1*OH	+	1*O	>	1*H	+	1*O2	1.38500E+13	0.0000	0.00	
17	1*O	+	1*H2	>	1*OH	+	1*H	3.38500E+11	0.0000	0.00	
18	1*OH	+	1*H	>	1*O	+	1*H2	3.83100E+11	0.0000	0.00	
19	1*O	+	1*H2O	>	2*OH			1.65000E+10	0.0000	0.00	
20			2*OH	>	1*O	+	1*H2O	4.10800E+12	0.0000	0.00	
21	1*H2O	+	1*H	>	1*OH	+	1*H2	7.70900E+09	0.0000	0.00	
22	1*OH	+	1*H2	>	1*H2O	+	1*H	1.83700E+12	0.0000	0.00	
23	1*OH	+	1*H2O2	>	1*H2O	+	1*H2O	3.63200E+12	0.0000	0.00	
24	1*H2O	+	1*H2O2	>	1*OH	+	1*H2O2	7.10700E+06	0.0000	0.00	
25	1*O	+	1*H2O2	>	1*OH	+	1*O2	2.16800E+13	0.0000	0.00	
26	1*OH	+	1*O2	>	1*O	+	1*H2O	2.47500E+02	0.0000	0.00	
27	1*H	+	1*H2O2	>	2*OH			1.12600E+14	0.0000	0.00	
28			2*OH	>	1*H	+	1*H2O	1.38500E+05	0.0000	0.00	
29	1*H	+	1*H2O2	>	1*H2	+	1*O2	2.50600E+13	0.0000	0.00	
30	1*H2	+	1*O2	>	1*H	+	1*H2O	2.48700E+02	0.0000	0.00	
31	1*H2O2	+	1*OH	>	1*H2O	+	1*O2	1.31300E+13	0.0000	0.00	
32	1*H2O	+	1*O2	>	1*H2O2	+	1*OH	5.52900E-01	0.0000	0.00	
33	1*O2	+	1*H2O2	>	2*H2O			1.34900E+05	0.0000	0.00	
34			2*H2O2	>	1*O2	+	1*H2O2	6.32400E+12	0.0000	0.00	
35	1*H2O2	+	1*H2	>	1*H2O2	+	1*H	1.40300E+08	0.0000	0.00	
36	1*H2O2	+	1*H	>	1*H2O2	+	1*H2	3.05400E+11	0.0000	0.00	
37	M	+	1*O2	>	2*O			2.03000E-08	0.0000	0.00	
38			2*O	>	1*O2	+	M	1.86100E+14	0.0000	0.00	
39	M	+	1*H2	>	2*H			1.85000E-05	0.0000	0.00	
40			2*H	>	1*H2	+	M	3.00000E+15	0.0000	0.00	
41	M	+	1*OH	>	1*O	+	1*H	1.80700E-04	0.0000	0.00	
42	1*O	+	1*H	>	1*OH	+	M	1.00100E+16	0.0000	0.00	
43	M	+	1*H2O2	>	2*OH			1.09000E+08	0.0000	0.00	
44			2*OH	>	1*H2O2	+	M	9.25100E+15	0.0000	0.00	
45	M	+	1*H2O	>	1*H	+	1*OH	3.01200E-05	0.0000	0.00	
46	1*H	+	1*OH	>	1*H2O	+	M	1.15700E+17	0.0000	0.00	
47	M	+	1*H2O2	>	1*H	+	1*O2	1.75300E+06	0.0000	0.00	
48	1*H	+	1*O2	>	1*H2O2	+	M	2.60500E+15	0.0000	0.00	
49	M	+	1*CO2	>	1*CO	+	1*O	3.23400E-08	0.0000	0.00	
50	1*CO	+	1*O	>	1*CO2	+	M	9.06700E+14	0.0000	0.00	
51	M	+	1*HCO	>	1*H	+	1*CO	2.77700E+10	0.0000	0.00	
52	1*H	+	1*CO	>	1*HCO	+	M	3.21000E+14	0.0000	0.00	

ALL THIRD BODY RATIOS ARE 1.0

TABLE E.2.—Continued.
(f) Continued.

** INITIAL CONDITIONS **									
TIME	0.00000E+00	SEC	AREA	0.00000E+00	SQ CM	AXIAL POSITION	0.00000E+00	CM	
FLOW PROPERTIES					INTEGRATION INDICATORS				
PRESSURE	1.00000		STEPS FROM LAST PRINT	0					
(ATM)			AVERAGE STEP SIZE	0.00000E+00					
VELOCITY	0.00		METHOD ORDER	0					
(CM/SEC)									
DENSITY	3.10486E-04		TOTAL NUMBER OF STEPS	0					
(G/CM**3)			FUNCT EVALUATIONS	0					
TEMPERATURE	1100.00		JACOBIAN EVALUATIONS	0					
(DEG K)									
MASS FLOW RATE	0.00000E+00								
(G/SEC)									
ENTROPY	1.9901								
(CAL/G/DEG K)									
MACH NUMBER	0.0000								
GAMMA	1.3319								
ENTHALPY	1.89467E+02								
(CAL/G)									
SP. HEAT (CP)	2.84564E-01								
(CAL/G/DEG K)									
CHEMICAL PROPERTIES									
SPECIES	CONCENTRATION	MOLE FRACTION	NET SPECIES PRODUCTION	REACTION	RATE CONST	NET REACTION CONV RATE	NET RATE/POSTI-		
	(MOLES/CM**3)		RATE (MOLE/CM**3/SEC)	NUMBER	CGS UNITS	(MOLE-CM**3/G**2/SEC)	TIVE DIR RATE		
HCO	0.00000E+00	0.00000E+00	8.97491E-21	1	2.0000E+14	0.00000E+00	0.00000		
H	0.00000E+00	0.00000E+00	3.69700E-17	2	1.7160E-03	0.00000E+00	0.00000		
CO	2.21578E-08	2.00000E-03	-5.83703E-12	3	1.0000E+14	0.00000E+00	0.00000		
HI2	0.00000E+00	0.00000E+00	0.00000E+00	4	3.6560E-06	9.30990E-14	1.00000		
OH	0.00000E+00	0.00000E+00	1.90389E-14	5	3.0120E+13	0.00000E+00	0.00000		
H2O	1.10789E-07	1.00000E-02	-1.90389E-14	6	2.8670E-04	0.00000E+00	0.00000		
O	0.00000E+00	0.00000E+00	5.83703E-12	7	3.0150E+12	0.00000E+00	0.00000		
O2	5.10209E-07	2.80000E-02	-5.85603E-12	8	2.5900E+06	0.00000E+00	0.00000		
HO2	0.00000E+00	0.00000E+00	1.90020E-14	9	3.0840E+09	0.00000E+00	0.00000		
CO2	0.00000E+00	0.00000E+00	5.83703E-12	10	1.7770E-02	0.00000E+00	0.00000		
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	11	1.9210E+11	0.00000E+00	0.00000		
N2	1.06358E-05	9.60000E-01	5.21115E-11	12	7.8900E+08	0.00000E+00	0.00000		
				13	4.4540E+02	0.00000E+00	0.00000		
				14	8.4920E+02	6.05490E-05	1.00000		
				15	1.1260E+11	0.00000E+00	0.00000		
				16	1.3850E+13	0.00000E+00	0.00000		
				17	3.3850E+11	0.00000E+00	0.00000		
				18	3.8310E+11	0.00000E+00	0.00000		
				19	1.6500E+10	0.00000E+00	0.00000		
				20	4.1080E+12	0.00000E+00	0.00000		
				21	7.7090E+09	0.00000E+00	0.00000		
				22	1.8370E+12	0.00000E+00	0.00000		
				23	3.6320E+12	0.00000E+00	0.00000		
				24	7.1070E+06	0.00000E+00	0.00000		
				25	2.1680E+13	0.00000E+00	0.00000		
				26	2.4750E+02	0.00000E+00	0.00000		
				27	1.1260E+14	0.00000E+00	0.00000		
				28	1.3850E+05	0.00000E+00	0.00000		
				29	2.5060E+13	0.00000E+00	0.00000		
				30	2.4870E+02	0.00000E+00	0.00000		
				31	1.3130E+13	0.00000E+00	0.00000		
				32	5.5290E-01	1.97112E-07	1.00000		
				33	1.5490E+05	0.00000E+00	0.00000		
				34	6.3240E+12	0.00000E+00	0.00000		
				35	1.4030E+08	0.00000E+00	0.00000		
				36	3.0560E+11	0.00000E+00	0.00000		
				37	2.0300E-08	7.23707E-13	1.00000		
				38	1.8610E+14	0.00000E+00	0.00000		
				39	1.8500E-05	0.00000E+00	0.00000		
				40	3.0000E+15	0.00000E+00	0.00000		
				41	1.8070E-04	0.00000E+00	0.00000		
				42	1.0010E+16	0.00000E+00	0.00000		
				43	1.0900E+08	0.00000E+00	0.00000		
				44	9.2510E+15	0.00000E+00	0.00000		
				45	3.0120E-05	3.83498E-10	1.00000		
				46	1.1570E+17	0.00000E+00	0.00000		
				47	1.7530E+06	0.00000E+00	0.00000		
				48	2.6050E+15	0.00000E+00	0.00000		
				49	3.2340E-08	0.00000E+00	0.00000		
				50	9.0690E+14	0.00000E+00	0.00000		
				51	2.7770E+10	0.00000E+00	0.00000		
				52	3.2100E+14	0.00000E+00	0.00000		
DERIVATIVES (CGS UNITS): T	0.00000E+00	RHD	0.00000E+00						
MIXTURE MOLECULAR HEIGHT	28.02500	TOTAL ENERGY EXCHANGE RATE	-4.75754E-01	MASS FRACTION SUM	1.00000000				
		(CAL-CM**3/G**2/SEC)							
CPU TIME FOR INITIALIZATION OF LSENS =	1.150001	S							

TABLE E.2.—Continued.
(f) Continued.

TIME	1.00000E+02	SEC	AREA	0.00000E+00	SQ CM	AXIAL POSITION	0.00000E+00	CM
FLOW PROPERTIES			INTEGRATION INDICATORS					
PRESSURE (ATM)	0.99900		STEPS FROM LAST PRINT	98				
VELOCITY (CM/SEC)	0.00		AVERAGE STEP SIZE	0.11394E+01				
DENSITY (G/CM**3)	3.10486E-04		METHOD ORDER	2				
TEMPERATURE (DEG K)	1100.00							
MASS FLOW RATE (G/SEC)	0.00000E+00		TOTAL NUMBER OF STEPS	183				
ENTROPY (CAL/G/DEG K)	1.9884		FUNCT EVALUATIONS	233				
MACH NUMBER	0.0000		JACOBIAN EVALUATIONS	31				
GAMMA	1.3313							
ENTHALPY (CAL/G)	1.84654E+02							
SP. HEAT (CP) (CAL/G/DEG K)	2.84633E-01							
CHEMICAL PROPERTIES								
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POSITIVE DIR	POSITIVE DIR RATE
HCO	1.40292E-30	1.26756E-25	8.48901E-30	1	2.0000E+14	6.75891E-21	1.00000	1.00000
H	2.32220E-18	2.09816E-13	1.09046E-19	2	1.7160E-03	2.19707E-27	1.00000	1.00000
CO	1.55444E-16	1.40446E-11	-3.18356E-21	3	1.0000E+14	1.97886E-21	1.00000	1.00000
H2	7.94032E-16	7.17423E-11	-9.52088E-21	4	3.6560E-06	6.53113E-22	1.00000	1.00000
OH	1.35978E-12	1.22859E-07	-1.75355E-17	5	3.0120E+13	1.82133E-24	1.00000	1.00000
H2O	1.10788E-07	1.00099E-02	8.60489E-18	6	2.8670E-04	6.28613E-25	1.00000	1.00000
D	4.15515E-15	3.75426E-10	4.99908E-18	7	3.0150E+12	1.31248E-17	1.00000	1.00000
O2	2.99130E-07	2.70270E-02	1.85412E-18	8	2.5900E+06	4.25933E-18	1.00000	1.00000
H02	1.02866E-15	9.29411E-11	-1.56016E-20	9	3.0840E+09	5.11531E-15	1.00000	1.00000
CO2	2.21578E-08	2.00200E-03	3.18356E-21	10	1.7770E-02	5.55389E-15	1.00000	1.00000
H2O2	1.56956E-16	1.41813E-11	1.25657E-19	11	1.9210E+11	4.21195E-10	1.00000	1.00000
H2	1.06358E-05	9.60961E-01	5.21113E-11	12	7.8900E+08	4.21133E-10	1.00000	1.00000
				13	4.4340E+02	4.25471E-13	1.00000	1.00000
				14	8.4920E+02	4.09598E-13	1.00000	1.00000
				15	1.1260E+11	8.11360E-07	1.00000	1.00000
				16	1.3850E+13	8.11744E-07	1.00000	1.00000
				17	3.3850E+11	1.15850E-11	1.00000	1.00000
				18	3.8310E+11	1.25486E-11	1.00000	1.00000
				19	1.6500E+10	7.87915E-05	1.00000	1.00000
				20	4.1080E+12	7.87919E-05	1.00000	1.00000
				21	7.7090E+09	2.05735E-08	1.00000	1.00000
				22	1.8370E+12	2.05745E-08	1.00000	1.00000
				23	3.6320E+12	8.04095E-09	1.00000	1.00000
				24	7.1070E+06	8.40167E-09	1.00000	1.00000
				25	2.1680E+13	9.61237E-10	1.00000	1.00000
				26	2.4750E+02	1.04428E-09	1.00000	1.00000
				27	1.1260E+14	2.79012E-12	1.00000	1.00000
				28	1.3850E+05	2.65644E-12	1.00000	1.00000
				29	2.5060E+13	6.20964E-13	1.00000	1.00000
				30	2.4870E+02	6.12758E-13	1.00000	1.00000
				31	1.3130E+13	1.90510E-07	1.00000	1.00000
				32	5.5290E-01	1.90071E-07	1.00000	1.00000
				33	1.3490E+05	6.57000E-11	1.00000	1.00000
				34	6.3240E+12	6.94140E-11	1.00000	1.00000
				35	1.4030E+08	1.18872E-15	1.00000	1.00000
				36	3.0540E+11	1.15468E-15	1.00000	1.00000
				37	2.0300E-08	6.97162E-13	1.00000	1.00000
				38	1.8610E+14	3.68890E-13	1.00000	1.00000
				39	1.8500E-05	1.68650E-18	1.00000	1.00000
				40	3.0000E+15	1.85737E-18	1.00000	1.00000
				41	1.8070E-04	2.82100E-14	1.00000	1.00000
				42	1.0010E+16	1.10891E-14	1.00000	1.00000
				43	1.0900E+08	1.96419E-06	1.00000	1.00000
				44	9.2510E+15	1.96382E-06	1.00000	1.00000
				45	3.0120E-05	3.83113E-10	1.00000	1.00000
				46	1.1570E+17	4.19449E-11	1.00000	1.00000
				47	1.7530E+06	2.07028E-07	1.00000	1.00000
				48	2.6050E+15	2.07752E-07	1.00000	1.00000
				49	3.2340E-08	8.22705E-14	1.00000	1.00000
				50	9.0690E+14	6.72506E-14	1.00000	1.00000
				51	2.7770E+10	4.47286E-18	1.00000	1.00000
				52	3.2100E+14	1.33032E-17	1.00000	1.00000
DERIVATIVES (CGS UNITS): T	0.00000E+00	RHO	0.00000E+00					
MIXTURE MOLECULAR WEIGHT	28.05305	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	-3.89288E-06	MASS FRACTION SUM	1.00000000			

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 5.450001E+00 S UP TO THIS TIME - 1.033000E+01 S

TABLE E.2.—Continued.
(f) Concluded.

```

***** SENSITIVITY CALCULATIONS *****
TIME = 1.00000D+02
SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

**** SENSITIVITY TO INITIAL CONDITIONS ****
DZ(I)/DYZERO(J)*F(J)/Z(I), WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
F(J)= YZERO(J) FOR YZERO(J) NOT EQUAL TO 0
      = 1.0E-4/(INITIAL MHT) FOR YZERO(J) = 0

PARAMETER   C0      H2
HCO          5.251D-02 5.630D-03
H            4.574D-03 2.647D-03
OH           2.355D-03 2.604D-03
O            1.645D-03 -2.698D-03
H02          -1.255D-03 3.517D-03
H2O2         1.232D-03 7.597D-03

TIME = 1.00000E+02

*** REACTION IMPORTANCE FOR NORMALIZED SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF Y(I) WRT PREEXPONENTIAL CONSTANTS ***

VARIABLE      REACTION NUMBER
NORMALIZED SENSITIVITY COEFFICIENT

C0
    11      12      16      15      20      19      31      32      48      47
-9.989E-01  9.988E-01  5.121E-01 -5.119E-01  5.104E-01 -5.104E-01 -4.963E-01  4.949E-01 -4.867E-01  4.847E-01
    24      23      43      44      26      25      45      13      14      46
1.426E-02 -1.366E-02  1.360E-02 -1.359E-02  2.727E-03 -2.711E-03  1.894E-03  1.005E-03 -9.717E-04 -2.077E-04
    49      50      34      33      10      9      27      28      37      22
1.955E-04 -1.598E-04 -6.284E-05  5.963E-05  1.519E-05 -1.213E-05 -8.980E-06  8.614E-06  5.012E-06 -2.838E-06
    21      29      38      30      41      18      17      42      36      35
2.762E-06 -1.626E-06 -1.597E-06  1.596E-06  1.597E-07  8.708E-08 -7.433E-08 -5.643E-08 -2.069E-09  2.022E-09
    52      51      7      40      3      39      8      1      5      4
-1.972E-09  4.891E-10 -4.622E-10 -6.291E-11 -2.144E-11  8.742E-12  4.922E-12 -4.040E-12 -1.261E-12  2.117E-13
    6      2
2.071E-18  9.892E-21

H2
    22      21      16      15      20      19      31      32      48      47
-9.994E-01  9.994E-01  5.131E-01 -5.129E-01  5.101E-01 -5.101E-01 -4.966E-01  4.955E-01 -4.868E-01  4.850E-01
    24      23      43      44      26      25      45      18      17      46
1.426E-02 -1.365E-02  1.359E-02 -1.359E-02  2.728E-03 -2.712E-03  1.896E-03  6.096E-04 -5.628E-04 -2.076E-04
    34      11      33      29      30      27      28      37      38      49
-6.319E-05 -6.163E-05  5.974E-05  2.855E-05 -2.817E-05 -9.05E-06  8.621E-06  3.013E-06 -1.596E-06  4.074E-07
    50      14      13      12      41      35      36      42      9      10
-5.636E-07 -2.775E-07  2.673E-07 -2.511E-07  1.598E-07 -5.773E-08  5.420E-08 -5.404E-08 -2.601E-08  1.801E-08
    52      51      7      40      39      3      1      8      5      4
-1.298E-09 -3.190E-10  3.005E-10  1.179E-10 -7.357E-11  1.771E-11  2.775E-12  1.315E-12  8.662E-13  2.090E-13
    6      2
2.024E-18 -1.012E-19

(LSENS)      END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:
TOTAL NO. OF STEPS - 183
TOTAL NO. OF DERIVATIVE EVALUATIONS - 233
TOTAL NO. OF JACOBIAN EVALUATIONS - 31
TOTAL CPU TIME - 10.330002 S

WORK REQUIRED BY SENSITIVITY ROUTINE:
NO. STEPS = 183
NO. FUNC. EVAL. = 183
NO. JAC. EVAL. = 183
TOTAL REAL SPACE USED = 4264
TOTAL INTEGER SPACE USED = 42

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 12.240001 S

(LSENS)      READ DATA FOR NEXT CASE

```


(g) Case 7

```
CC      1          2          3          4          5          6          7          8  
       123456789012345678901234567890123456789012345678901234567890
```

```
** DATA LINES **  
NEW     SIMPLE NONISOTHERMAL TEST CASE   R>P                                CASE 7  
DUMR    > DUMP                               1.0    1.0                0.0  
- BLANK LINE -  
- BLANK LINE -  
TIME     PRESSURE  
        &prob pcon=.true., sencal=.true., senstd=.true.,  
           print=1.0E+06,i.1.E+04,l.1.E+02,, &iend &sensd  
        &start t=1000.0,p=1.0, &iend  
DUMR     1.00  
END  
&solver emax=1.0E-3, atolsp=1.0E-12, &iend  
INIT  
ALL      END  
SENSVAR  ALL  
REAC     END  
         &sonrxn sensaj=.true., sensnj=.true., sensej=.true., allrxn=.true.,  
         &iend  
FINISH
```

```

** INITIAL CONDITIONS **
TIME      0.000000E+00 SEC      AREA  0.000000E+00 SQ CM      AXIAL POSITION  0.000000E+00 CM

```

FLOW PROPERTIES

PRESSURE (ATM)	1.00000
VELOCITY (CM/SEC)	0.00
DENSITY (G/CM**3)	1.21868E-05
TEMPERATURE (DEG K)	1000.00
MASS FLOW RATE (G/SEC)	0.00000E+00
ENTROPY (CAL/G/DEG K)	34.5388
MACH NUMBER	0.0000
GAMMA	1.6596
ENTHALPY (CAL/G)	5.00000E+03
SP. HEAT (CP) (CAL/G/DEG K)	5.00000E+00

INTEGRATION INDICATORS

STEPS FROM LAST PRINT	0
AVERAGE STEP SIZE	0.00000E+00
METHOD ORDER	0
TOTAL NUMBER OF STEPS	0
FUNCT EVALUATIONS	0
JACOBIAN EVALUATIONS	0

CHEMICAL PROPERTIES

SPECIES	CONCENTRATION (MOLE-CM ³)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE-CM ³ /SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM ³ /GMR ² /SEC)	NET RATE/POSITIVE DIR RATE
DUMP	1.21868E-05	1.00000E+00	-1.21868E-02	1	1.0000E+03	8.20560E+07	1.00000
DUMP	0.00000E+00	0.00000E+00	1.21868E-02				

DERIVATIVES (CGS UNITS): T	1.00000E+06	RHO	-1.21868E-02
----------------------------	-------------	-----	--------------

MIXTURE MOLECULAR HEIGHT	1.00000	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)	-4.10280E+11	MASS FRACTION SUM	1.00000000
--------------------------	---------	--	--------------	-------------------	------------

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CPU TIME FOR INITIALIZATION OF LSENS =      0.359999 S

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TABLE E.2.—Continued.
(g) Continued.

TIME	1.00000E-02	SEC	AREA	0.00000E+00	SQ CM	AXIAL POSITION	0.00000E+00	CM
FLOW PROPERTIES					INTEGRATION INDICATORS			
PRESSURE (ATM)	1.00000		STEPS FROM LAST PRINT			69		
VELOCITY (CM/SEC)	0.00		AVERAGE STEP SIZE			0.14541E-03		
DENSITY (G/CM**3)	6.09842E-06		METHOD ORDER			4		
TEMPERATURE (DEG K)	2000.00		TOTAL NUMBER OF STEPS			84		
MASS FLOW RATE (G/SEC)	0.00000E+00		FUNCT EVALUATIONS			101		
ENTROPY (CAL/G/DEG K)	38.0045		JACOBIAN EVALUATIONS			13		
MACH NUMBER	0.0000							
GAMMA	1.6596							
ENTHALPY (CAL/G)	5.00000E+03							
SP. HEAT (CP) (CAL/G/DEG K)	5.00000E+00							
CHEMICAL PROPERTIES								
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE/CM**3/G**2/SEC)	NET RATE/POSITIVE DIR RATE	
DUMR	2.47386E-14	4.05656E-09	-4.94773E-11	1	2.0000E+03	1.35036E+00	1.00000	
DUMP	6.09842E-06	1.00000E+00	4.94773E-11					
DERIVATIVES (CGS UNITS): T			8.11312E-03	RHO	-2.47386E-11			
MIXTURE MOLECULAR WEIGHT		1.00000	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)		-6.65182E+03	MASS FRACTION SUM		1.00000000

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 3.199997E-01 S UP TO THIS TIME - 4.000015E-01 S

***** SENSITIVITY CALCULATIONS *****

TIME = 1.00000E-02

SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

**** SENSITIVITY TO INITIAL CONDITIONS ****

DZ(I)/DYZERO(J)*F(J)/Z(I), WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
F(J)= YZERO(J) FOR YZERO(J) NOT EQUAL TO 0
= 1.0E-4/(INITIAL MNT) FOR YZERO(J) = 0

PARAMETER	DUMR	DUMP	TEMP	DENSITY
DUMR	1.0020+00	1.0000+00	-2.9520-05	2.9760-05
DUMP	9.5530-04	1.0000-04	-5.0000-05	4.9900-05
TEMP	-1.0540+01	4.2750-08	5.0000-01	4.9850-01
DENSITY	0.0000+00	0.0000+00	0.0000+00	1.0000+00

**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS ****

DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

REAC NUM	DUMR	DUMP	TEMP	DENSITY
1	-2.0090+01	8.1500-08	4.0750-08	-4.5200-04

**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE TEMPERATURE EXPONENTS ****

DZ(I)/DN(J)/(Z(I)*LN(T0)) WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

REAC NUM	DUMR	DUMP	TEMP	DENSITY
1	-2.1990+01	8.9200-08	4.4600-08	-3.8990-04

**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE ACTIVATION ENERGIES ****

DZ(I)/DE(J)*(1-RT0/Z(I)), WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

REAC NUM	DUMR	DUMP	TEMP	DENSITY
1	-1.0540+01	4.2750-08	2.1380-08	-7.4950-04

TABLE E.2.—Continued.
(g) Concluded.

```

***** SENSITIVITY CALCULATIONS *****
TIME = 1.00000D-02
SENSITIVITY COEFFICIENTS OF 1-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

**** SENSITIVITY TO INITIAL CONDITIONS ****
DZ(I)/DYZERO(J)*F(J)/Z(I), WHERE Z(I)= 1-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
F(J)= YZERO(J) FOR YZERO(J) NOT EQUAL TO 0
= 1.0E-4/(INITIAL UNIT) FOR YZERO(J) = 0

PARAMETER    DUMR    DUMP    TEMP    DENSITY
DUMR          1.002D+00  1.002D+00  1.635D-03  1.694D-03
DUMP          9.037D-04  9.037D-04  8.037D-04  9.036D-04
TEMP         -1.002D+01 -1.002D+01 -1.002D+01 -1.002D+01
DENSITY       0.000D+00  0.000D+00  0.000D+00  1.000D+00

**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS ****
DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 1-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

REAC NUM      DUMR      DUMP      TEMP      DENSITY
1             -1.906D+01 -1.906D+01 -1.906D+01 -1.906D+01

**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE TEMPERATURE EXPONENTS ****
DZ(I)/DN(J)/[Z(I)*LN(T0)] WHERE Z(I)= 1-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

REAC NUM      DUMR      DUMP      TEMP      DENSITY
1             -2.086D+01 -2.086D+01 -2.086D+01 -2.086D+01

**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE ACTIVATION ENERGIES ****
DZ(I)/DE(J)*[1-R*T0/Z(I)], WHERE Z(I)= 1-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

REAC NUM      DUMR      DUMP      TEMP      DENSITY
1             -1.002D+01 -1.002D+01 -1.002D+01 -1.002D+01

(15ENS)      END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:
TOTAL NO. OF STEPS - 84
TOTAL NO. OF DERIVATIVE EVALUATIONS - 101
TOTAL NO. OF JACOBIAN EVALUATIONS - 13
TOTAL CPU TIME - 0.400002 S

WORK REQUIRED BY SENSITIVITY ROUTINE:
NO. STEPS = 84
NO. FUNC. EVAL. = 84
NO. JAC. EVAL. = 84
TOTAL REAL SPACE USED = 264
TOTAL INTEGER SPACE USED = 48

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 0.980000 S

(15ENS)      READ DATA FOR NEXT CASE

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TABLE E.2.—Continued.
(h) Case 8

TIME-PRESSURE VERSION			LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM					NASA LEWIS RESEARCH CENTER		
HYDROGEN COMBUSTION IN STANDARD AIR AT 3.10 ATM.							CASE 8			
REACTION NUMBER		REACTION			REACTION RATE VARIABLES A N		ACTIVATION ENERGY			
1	1*CO	+	1*O	=	1*CO2	+	M	5.88800E+15	0.0000	4100.00
2	1*CO	+	1*O2	=	1*CO2	+	1*O	2.51200E+12	0.0000	47690.00
3	1*CO	+	1*OH	=	1*CO2	+	1*H	4.16900E+11	0.0000	1000.00
4	1*CO	+	1*HO2	=	1*CO2	+	1*OH	5.75400E+13	0.0000	22930.00
5	1*O	+	1*H2O	=	2*OH			6.80000E+13	0.0000	18365.00
6	1*H	+	1*O2	=	1*OH	+	1*O	1.89000E+14	0.0000	16400.00
7	1*O	+	1*H2	=	1*OH	+	1*H	4.20000E+14	0.0000	13750.00
8	1*H	+	1*HO2	=	1*H2	+	1*O2	7.28000E+13	0.0000	2126.00
9	1*O	+	1*HO2	=	1*OH	+	1*O2	5.00000E+13	0.0000	1000.00
10	1*HO2	+	1*OH	=	1*H2O	+	1*O2	8.00000E+12	0.0000	0.00
11	1*H	+	1*HO2	=	2*OH			1.34000E+14	0.0000	1070.00
12	1*H2	+	1*HO2	=	1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00
13	1*OH	+	1*H2O2	=	1*H2O	+	1*HO2	6.10000E+12	0.0000	1430.00
14			2*H2O2	=	1*H2O2	+	1*O2	1.80000E+12	0.0000	0.00
15	1*H	+	1*H2O2	=	1*OH	+	1*H2O	7.80000E+11	0.0000	0.00
16	M	+	1*H2O2	=	2*OH			1.44000E+17	0.0000	45510.00
17	1*H2	+	1*OH	=	1*H2O	+	1*H	4.74000E+13	0.0000	6098.00
18	1*H	+	1*O2	=	1*HO2	+	M	1.46000E+15	0.0000	-1000.00
19	M	+	1*H2O	=	1*H	+	1*OH	1.30000E+15	0.0000	105140.00
20	1*H	+	1*O	=	1*OH	+	M	7.10000E+18	-1.0000	0.00
21	M	+	1*H2	=	2*H			2.20000E+14	0.0000	96000.00
22	M	+	1*O2	=	2*O			1.80000E+18	-1.0000	118020.00
23	1*HO2	+	1*HO	=	1*NO2	+	1*OH	2.09000E+12	0.0000	-477.00
24	1*O	+	1*HO2	=	1*HO	+	1*O2	1.00000E+13	0.0000	596.00
25	1*HO	+	1*O	=	1*NO2	+	M	5.62000E+15	0.0000	-1160.00
26	1*HO2	+	1*H	=	1*HO	+	1*OH	3.47000E+14	0.0000	1470.00
27	1*HO	+	1*O	=	1*H	+	1*O2	3.80000E+09	1.0000	41370.00
28	1*O	+	1*H2	=	1*H	+	1*H	1.80000E+14	0.0000	76250.00
29	1*HO	+	1*H	=	1*H	+	1*OH	2.63000E+14	0.0000	50410.00
30	M	+	1*H2O	=	1*H2	+	1*O	6.92000E+23	-2.5000	65000.00
31	1*O	+	1*H2O	=	1*H2	+	1*O2	1.00000E+14	0.0000	28020.00
32	1*O	+	1*H2O	=	2*HO			6.92000E+13	0.0000	26630.00
33	1*H	+	1*HO2	=	2*HO			4.00000E+12	0.0000	0.00
34	1*H2O	+	1*H	=	1*H2	+	1*OH	7.59000E+13	0.0000	15100.00
35	1*HO2	+	1*H2	=	1*HHO2	+	1*H	2.40000E+13	0.0000	29000.00
36	1*OH	+	1*HO2	=	1*HHO3	+	M	3.00000E+15	0.0000	-3800.00
37	1*OH	+	1*HO	=	1*HHO2	+	M	5.60000E+15	0.0000	-1700.00
38	1*HHO	+	1*H	=	1*H2	+	1*HO	5.00000E+12	0.0000	0.00
39	1*H	+	1*HO	=	1*HHO	+	M	5.40000E+15	0.0000	-600.00
40	1*HHO	+	1*OH	=	1*H2O	+	1*NO	3.60000E+13	0.0000	0.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(H2	, 16) = 2.30000	M(O2	, 16) = 0.78000	M(H2O	, 16) = 6.00000	M(H2O2	, 16) = 6.60000
M(O2	, 18) = 1.30000	M(H2	, 18) = 1.30000	M(H2O	, 18) = 21.30000	M(H2	, 18) = 5.00000
M(H2	, 19) = 4.00000	M(O2	, 19) = 1.50000	M(H2O	, 19) = 20.00000	M(H2	, 19) = 1.50000
M(H2	, 21) = 4.10000	M(O2	, 21) = 2.00000	M(H2O	, 21) = 15.00000	M(H2	, 21) = 2.00000
M(O2	, 36) = 0.70000	M(H2	, 36) = 1.40000				

** INITIAL CONDITIONS **

TIME	0.00000E+00	SEC	AREA	0.00000E+00	SQ CM	AXIAL POSITION	0.00000E+00	CM
FLOW PROPERTIES					INTEGRATION INDICATORS			
PRESSURE (ATM)	3.10000					STEPS FROM LAST PRINT	0	
VELOCITY (CM/SEC)	0.00					AVERAGE STEP SIZE	0.00000E+00	
DENSITY (G/CM**3)	8.35179E-04					METHOD ORDER	0	
TEMPERATURE (DEG K)	950.66							
MASS FLOW RATE (G/SEC)	0.00000E+00					TOTAL NUMBER OF STEPS	0	
ENTROPY (KCAL/G/DEG K)	2.3811					FUNCT EVALUATIONS	0	
MACH NUMBER	0.0000					JACOBIAN EVALUATIONS	0	
GAMMA	1.3514							
ENTHALPY (CAL/G)	2.28819E+02							
SP. HEAT (CP) (CAL/G/DEG K)	5.63657E-01							

TABLE E.2.—Continued.
(h) Continued.

CHEMICAL PROPERTIES							
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	HIT RATE/POST- TIVE DIR RATE
CO	0.00000E+00	0.00000E+00	9.55759E-25	1	6.7206E+14	-1.37022E-18	1.00000
O	0.00000E+00	0.00000E+00	4.21098E-11	2	2.7317E+01	0.00000E+00	0.00000
CO2	8.40100E-09	2.11400E-04	-9.55759E-25	3	2.4555E+11	0.00000E+00	0.00000
O2	5.86721E-06	1.47640E-01	-3.39182E-09	4	3.0799E+08	0.00000E+00	0.00000
OH	0.00000E+00	0.00000E+00	0.00000E+00	5	4.0788E+09	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	3.35098E-09	6	3.2079E+10	0.00000E+00	0.00000
H02	0.00000E+00	0.00000E+00	3.34971E-09	7	2.8988E+11	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	0.00000E+00	8	2.3625E+13	-4.80228E-03	1.00000
H2	1.17341E-05	2.95273E-01	-3.35098E-09	9	2.9449E+13	0.00000E+00	0.00000
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	10	8.0000E+12	0.00000E+00	0.00000
H0	1.78829E-07	4.50000E-03	-4.33823E-11	11	7.6054E+13	0.00000E+00	0.00000
H02	0.00000E+00	0.00000E+00	4.21096E-11	12	1.4153E+08	0.00000E+00	0.00000
H	0.00000E+00	0.00000E+00	7.51490E-21	13	2.8614E+12	0.00000E+00	0.00000
H2	2.16903E-05	5.45807E-01	-6.35262E-22	14	1.8000E+12	0.00000E+00	0.00000
H2O	0.00000E+00	0.00000E+00	1.21953E-16	15	7.8000E+11	0.00000E+00	0.00000
H102	0.00000E+00	0.00000E+00	0.00000E+00	16	4.9653E+06	0.00000E+00	0.00000
H103	0.00000E+00	0.00000E+00	0.00000E+00	17	1.8789E+12	0.00000E+00	0.00000
H10	0.00000E+00	0.00000E+00	1.27237E-12	18	2.4788E+15	0.00000E+00	0.00000
AR	2.61013E-07	6.56810E-03	0.00000E+00	19	8.7705E-10	0.00000E+00	0.00000
				20	7.4685E+15	0.00000E+00	0.00000
				21	1.8738E-08	3.26794E-11	1.00000
				22	1.3974E-12	4.67100E-16	1.00000
				23	2.6903E+12	0.00000E+00	0.00000
				24	7.2943E+12	-6.03702E-05	1.00000
				25	1.0385E+16	0.00000E+00	0.00000
				26	1.5936E+14	0.00000E+00	0.00000
				27	1.1147E+103	0.00000E+00	0.00000
				28	5.3205E-04	0.00000E+00	0.00000
				29	6.7774E+02	0.00000E+00	0.00000
				30	2.8315E+01	0.00000E+00	0.00000
				31	3.6175E+07	-9.10738E-16	1.00000
				32	5.2247E+07	-1.74836E-10	1.00000
				33	4.0000E+12	-1.07737E-14	1.00000
				34	2.5637E+10	0.00000E+00	0.00000
				35	5.1680E+06	0.00000E+00	0.00000
				36	2.2424E+16	0.00000E+00	0.00000
				37	1.3772E+16	0.00000E+00	0.00000
				38	5.0000E+12	-1.82412E-06	1.00000
				39	7.4187E+15	0.00000E+00	0.00000
				40	3.6000E+13	0.00000E+00	0.00000
DERIVATIVES (CGS UNITS): T			-5.8848E-01	RHO	5.17001E-07		
MIXTURE MOLECULAR WEIGHT		21.01616	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/G**2/SEC)		2.55482E+02	MASS FRACTION SUM	1.00000000
CPU TIME FOR INITIALIZATION OF LSENS =					1.260000 S		

TIME	2.00000E-04 SEC	AREA	0.00000E+00 SQ CM	AXIAL POSITION	0.00000E+00 CM
FLOW PROPERTIES			INTEGRATION INDICATORS		
PRESSURE (ATM)	3.10000	STEPS FROM LAST PRINT		132	
VELOCITY (CM/SEC)	0.00	AVERAGE STEP SIZE		0.15001E-06	
DENSITY (G/CM**3)	3.51245E-04	METHOD ORDER		3	
TEMPERATURE (DEG K)	2541.16				
MASS FLOW RATE (G/SEC)	0.00000E+00	TOTAL NUMBER OF STEPS		228	
ENTROPY (CAL/G/DEG K)	2.6303	FUNC EVALUATIONS		379	
MACH NUMBER	0.0000	JACOBIAN EVALUATIONS		39	
GAMMA	1.2550				
ENTHALPY (CAL/G)	2.28818E+02				
SP. HEAT (CP) (CAL/G/DEG K)	4.13930E-01				

TABLE E.2.—Continued.
(h) Continued.

CHEMICAL PROPERTIES							
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/GM**2/SEC)	NET RATE/POST- TIVE DIR RATE
CO	1.67166E-09	1.12439E-04	6.63430E-06	1	2.6143E+15	-4.41273E+01	0.95189
O	8.80256E-08	5.92079E-03	-4.92577E-03	2	1.9883E+08	-3.58042E-02	0.05288
CO2	1.86148E-09	1.25207E-04	-6.63430E-06	3	3.4200E+11	-9.94751E+01	0.05779
O2	2.38046E-07	1.60113E-02	-6.95371E-03	4	6.1362E+11	1.60922E+00	0.76161
OH	3.50002E-07	2.35419E-02	-4.81197E-03	5	1.7908E+12	-2.91878E+03	0.00057
H	2.40937E-07	1.62060E-02	-1.48576E-02	6	7.3451E+12	1.77058E+04	0.00519
H2O	2.54128E-10	1.70932E-05	-9.33737E-06	7	2.7586E+13	4.27096E+04	0.00352
H2	4.02200E-06	2.70528E-01	-2.36563E-02	8	4.7784E+13	1.83418E+04	0.77342
H2	6.17267E-07	4.15187E-02	-1.38113E-02	9	4.1017E+13	5.75800E+03	0.77472
H2O2	3.08090E-11	2.07228E-06	-5.37934E-06	10	8.0000E+12	4.46611E+03	0.77435
HO	7.51649E-08	5.05575E-03	2.46971E-05	11	1.0841E+14	4.17194E+04	0.77539
H2O2	1.68514E-11	1.13346E-06	3.36730E-07	12	5.5986E+11	-2.73562E+03	0.79352
H	1.14976E-11	7.73489E-07	2.63812E-07	13	4.5956E+12	3.19075E+02	0.79466
H2	9.12211E-06	6.13572E-01	-1.07127E-05	14	1.8000E+12	-9.16922E-02	0.08868
H2O	4.13216E-12	2.77938E-07	1.75265E-07	15	7.8000E+11	4.47630E+01	0.95381
HHO2	4.34027E-12	2.91936E-07	-3.94736E-07	16	1.7552E+15	-3.07215E+03	0.01924
HHO3	1.74341E-16	1.17265E-11	-1.69994E-11	17	1.4169E+13	1.01255E+05	0.00408
HHO	3.67249E-11	2.47019E-06	-3.82810E-06	18	1.7797E+15	6.73114E+04	0.79925
AR	1.09773E-07	7.38358E-03	0.00000E+00	19	1.1789E+06	-7.92304E+04	0.95470
				20	2.7940E+15	6.81717E+03	0.95467
				21	1.1911E+06	-1.05531E+04	0.95451
				22	5.0125E+04	-3.01206E+01	0.95444
				23	2.2970E+12	1.55126E+02	0.43618
				24	8.8867E+12	6.40614E+01	0.59956
				25	7.0713E+15	4.99663E+03	0.88622
				26	2.5936E+14	5.13517E+03	0.60163
				27	2.6720E+09	-6.85876E+00	0.04568
				28	4.9828E+07	8.46624E+01	0.26106
				29	1.2148E+10	-7.56614E+01	0.04070
				30	5.4610E+09	-2.13127E+01	0.88685
				31	3.8920E+11	6.85423E-01	0.59734
				32	3.5467E+11	7.48739E-01	0.71605
				33	4.0000E+12	3.88187E-03	0.61785
				34	3.8158E+12	1.84579E+01	0.59963
				35	7.6930E+10	-5.02127E+01	0.88560
				36	6.3670E+15	-1.37789E-04	0.00003
				37	7.8414E+15	4.70131E+01	0.00189
				38	5.0000E+12	3.35707E+02	0.93615
				39	6.0813E+15	3.81689E+03	0.28760
				40	3.6000E+13	3.51221E+03	0.93641
DERIVATIVES (CGS UNITS): T							
		1.77523E+07	RHO	-1.94094E+00			
MIXTURE MOLECULAR WEIGHT		23.62546	TOTAL ENERGY EXCHANGE RATE (CAL-CM**3/GM**2/SEC)		-2.0893E+10	MASS FRACTION SUM	1.00000010

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 9.860001E+00 S UP TO THIS TIME - 1.659000E+01 S

***** SENSITIVITY CALCULATIONS *****

TIME = 2.00000D-04

SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

**** SENSITIVITY TO INITIAL CONDITIONS ****

DZ(I)/DYZERO(J)*F(J)/Z(I), WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
F(J)= YZERO(J) FOR YZERO(J) NOT EQUAL TO 0
= 1.0E-4/(INITIAL MNT) FOR YZERO(J) = 0

PARAMETER	CO	CO2	OH	H2O	H2	HO	TEMP
CO	5.195D-01	4.313D-01	1.378D-04	-2.015D-04	9.540D-04	-9.365D-06	-1.229D-04
H2	1.336D+00	-1.199D+00	8.467D-01	1.506D-01	5.383D+00	-3.852D-02	-3.705D-01
O2	-8.292D-01	7.447D-01	3.077D-01	9.769D-01	-4.887D+00	6.952D-02	8.772D-01
H2O2	2.138D+03	-1.920D+03	-7.454D+03	3.176D+03	-1.209D+04	1.767D+02	3.770D+03
H2O2	1.562D+01	-1.403D+01	-5.446D+01	2.321D+01	-8.834D+01	1.291D+00	2.755D+01
HO	2.729D-01	-2.451D-01	-9.933D-01	4.218D-01	-1.605D+00	1.012D+00	4.977D-01
TEMP	1.108D+01	-9.946D+00	-3.656D+01	1.577D+01	-6.004D+01	8.958D-01	1.906D+01
DENSITY	-8.695D-02	7.808D-02	-2.351D-01	9.916D-02	-3.758D-01	4.545D-03	1.181D-01

TIME = 2.00000E-04

*** REACTION IMPORTANCE FOR NORMALIZED SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF Y(I) WRT PREEXPONENTIAL CONSTANTS ***

VARIABLE	REACTION NUMBER					
	NORMALIZED SENSITIVITY COEFFICIENT					
CO	6	18	8	11	17	5
	1.018E+00	-6.199E-01	-1.402E-01	1.182E-01	6.086E-02	6.243E-05
CO2	6	18	8	11	17	5
	-9.145E-01	5.567E-01	1.259E-01	-1.062E-01	-3.465E-02	-5.606E-05
OH	6	18	8	11	17	5
	-3.553E+00	1.982E+00	4.869E-01	-4.191E-01	-2.056E-01	1.257E-05

TABLE E.2.—Continued.
(h) Concluded.

	6	18	8	11	17	5
H2O	1.515E+00	-8.443E-01	-2.079E-01	1.794E-01	8.754E-02	-5.079E-05
H2	-5.766E+00	3.213E+00	7.919E-01	-6.835E-01	-3.338E-01	1.283E-04
HO	8.430E-02	-4.704E-02	-1.159E-02	9.979E-03	4.847E-03	-2.308E-06
TEMP	1.798E+00	-1.002E+00	-2.467E-01	2.128E-01	1.038E-01	-3.873E-05

*** REACTION IMPORTANCE FOR NORMALIZED SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF Y(I) WRT ACTIVATION ENERGIES ***

VARIABLE

REACTION NUMBER

NORMALIZED SENSITIVITY COEFFICIENT

	6	18	8	11	17	5
CO	9.973E-01	-5.887E-01	-1.316E-01	1.120E-01	5.767E-02	2.268E-05
CO2	-8.956E-01	5.286E-01	1.181E-01	-1.006E-01	-5.179E-02	-2.037E-05
OH	-3.478E+00	1.977E+00	4.579E-01	-3.933E-01	-1.981E-01	3.077E-05
H2O	1.482E+00	-8.421E-01	-1.953E-01	1.679E-01	8.438E-02	-2.263E-05
H2	-5.643E+00	3.205E+00	7.436E-01	-6.393E-01	-3.214E-01	9.026E-05
HO	8.249E-02	-4.686E-02	-1.087E-02	9.341E-03	4.685E-03	-1.573E-06
TEMP	1.759E+00	-9.995E-01	-2.318E-01	1.992E-01	1.001E-01	-2.767E-05

(LSENS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS - 228
TOTAL NO. OF DERIVATIVE EVALUATIONS - 379
TOTAL NO. OF JACOBIAN EVALUATIONS - 39
TOTAL CPU TIME - 16.590000 S

WORK REQUIRED BY SENSITIVITY ROUTINE:

NO. STEPS = 228
NO. FUNC. EVAL. = 228
NO. JAC. EVAL. = 228
TOTAL REAL SPACE USED = 3424
TOTAL INTEGER SPACE USED = 80

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 18.650002 S

(LSENS) READ DATA FOR NEXT CASE

TABLE E.2.—Continued.

(i) Case 9

LEWIS SENSITIVITY AND GENERAL KINETICS PROGRAM

NASA LEWIS RESEARCH CENTER

BENZENE-OXYGEN-AR SHOCK IGNITION - WITH SENSITIVITY MECHANISM K-70 CASE 9

REACTION NUMBER	REACTION						REACTION RATE VARIABLES		ACTIVATION ENERGY	
							A	N		
1	1* <chem>C6H6</chem>	+	1* <chem>O2</chem>	=	1* <chem>C6H5O</chem>	+	1* <chem>OH</chem>	4.00000E+13	0.0000	34000.00
2	1* <chem>C6H6</chem>	+	1* <chem>C6H5</chem>	=	1* <chem>C12H10</chem>	+	1* <chem>H</chem>	4.00000E+11	0.0000	4000.00
3			1* <chem>C6H6</chem>	=	1* <chem>C6H5</chem>	+	1* <chem>H</chem>	1.00000E+16	0.0000	108000.00
4	1* <chem>C6H6</chem>	+	1* <chem>H</chem>	=	1* <chem>C6H5</chem>	+	1* <chem>H2</chem>	2.50000E+14	0.0000	16000.00
5	1* <chem>C6H6</chem>	+	1* <chem>O</chem>	=	1* <chem>C6H5O</chem>	+	1* <chem>H</chem>	2.78300E+13	0.0000	4910.00
6	1* <chem>C6H6</chem>	+	1* <chem>OH</chem>	=	1* <chem>C6H5</chem>	+	1* <chem>H2O</chem>	2.13200E+13	0.0000	4580.00
7	M	+	1* <chem>C4H3</chem>	=	1* <chem>C4H2</chem>	+	1* <chem>H</chem>	1.00000E+16	0.0000	60000.00
8			1* <chem>C6H5O</chem>	=	1* <chem>C5H5</chem>	+	1* <chem>CO</chem>	2.51000E+11	0.0000	43900.00
9	1* <chem>C6H5</chem>	+	1* <chem>O2</chem>	=	1* <chem>C6H5O</chem>	+	1* <chem>O</chem>	2.10000E+12	0.0000	7470.00
10	1* <chem>C6H5</chem>	+	1* <chem>H2O2</chem>	=	1* <chem>C6H5O</chem>	+	1* <chem>OH</chem>	2.00000E+13	0.0000	1000.00
11			1* <chem>C6H5</chem>	=	1* <chem>C4H3</chem>	+	1* <chem>C2H2</chem>	4.50000E+13	0.0000	72530.00
12			1* <chem>C6H5OH</chem>	=	1* <chem>C6H5O</chem>	+	1* <chem>H</chem>	2.00000E+16	0.0000	88000.00
13	1* <chem>C6H5OH</chem>	+	1* <chem>H</chem>	=	1* <chem>C6H6</chem>	+	1* <chem>OH</chem>	2.20000E+13	0.0000	7910.00
14	1* <chem>C6H5OH</chem>	+	1* <chem>H</chem>	=	1* <chem>C6H5O</chem>	+	1* <chem>H2</chem>	1.15000E+14	0.0000	12405.00
15	1* <chem>C5H5</chem>	+	1* <chem>C6H5OH</chem>	=	1* <chem>C6H5O</chem>	+	1* <chem>C5H6</chem>	2.67000E+14	0.0000	25227.00
16			1* <chem>C5H6</chem>	=	1* <chem>C5H5</chem>	+	1* <chem>H</chem>	8.13000E+24	-2.9810	78682.00
17	1* <chem>C5H6</chem>	+	1* <chem>O2</chem>	=	1* <chem>C5H5O</chem>	+	1* <chem>OH</chem>	1.00000E+13	0.0000	20712.00
18	1* <chem>C6H5OH</chem>	+	1* <chem>OH</chem>	=	1* <chem>C6H5O</chem>	+	1* <chem>H2O</chem>	3.00000E+13	0.0000	0.00
19	1* <chem>C6H5OH</chem>	+	1* <chem>H2O2</chem>	=	1* <chem>C6H5O</chem>	+	1* <chem>H2O2</chem>	3.00000E+13	0.0000	1500.00
20			1* <chem>C5H5O</chem>	=	1* <chem>C4H5</chem>	+	1* <chem>CO</chem>	3.00000E+16	0.0000	15000.00
21	1* <chem>C5H5</chem>	+	1* <chem>O</chem>	=	1* <chem>C5H5O</chem>	+	1* <chem>H</chem>	1.00000E+13	0.0000	0.00
22	1* <chem>C5H5</chem>	+	1* <chem>OH</chem>	=	1* <chem>C5H4OH</chem>	+	1* <chem>H</chem>	1.00000E+13	0.0000	0.00
23			1* <chem>C5H4OH</chem>	=	1* <chem>C4H4</chem>	+	1* <chem>HCO</chem>	1.00000E+15	0.0000	22000.00
24	1* <chem>C5H5</chem>	+	1* <chem>H2O2</chem>	=	1* <chem>C5H5O</chem>	+	1* <chem>OH</chem>	2.00000E+13	0.0000	0.00
25			2* <chem>C6H5</chem>	=	1* <chem>C12H10</chem>	+		3.10000E+12	0.0000	0.00
26			1* <chem>C4H5</chem>	=	1* <chem>C2H3</chem>	+	1* <chem>C2H2</chem>	1.40000E+13	0.0000	32900.00
27	1* <chem>C4H2</chem>	+	1* <chem>O</chem>	=	1* <chem>C2H0</chem>	+	1* <chem>C2H</chem>	1.00000E+13	0.0000	0.00
28	1* <chem>C4H2</chem>	+	1* <chem>OH</chem>	=	1* <chem>HCO</chem>	+	1* <chem>C3H2</chem>	3.00000E+13	0.0000	0.00
29	1* <chem>C4H2</chem>	+	1* <chem>O</chem>	=	1* <chem>CO</chem>	+	1* <chem>C3H2</chem>	1.20000E+12	0.0000	0.00
30	M	+	1* <chem>C2H4</chem>	=	1* <chem>C2H2</chem>	+	1* <chem>H2</chem>	9.35000E+16	0.0000	77200.00
31	1* <chem>C2H4</chem>	+	1* <chem>OH</chem>	=	1* <chem>C2H3</chem>	+	1* <chem>H2O</chem>	4.78600E+12	0.0000	12330.00
32	1* <chem>C2H4</chem>	+	1* <chem>O</chem>	=	1* <chem>CH3</chem>	+	1* <chem>HCO</chem>	3.31100E+12	0.0000	11330.00
33	1* <chem>C2H4</chem>	+	1* <chem>O</chem>	=	1* <chem>CH2O</chem>	+	1* <chem>CH2</chem>	2.51200E+13	0.0000	5000.00
34	1* <chem>C2H4</chem>	+	1* <chem>OH</chem>	=	1* <chem>CH3</chem>	+	1* <chem>CH2O</chem>	1.99500E+12	0.0000	960.00
35	M	+	1* <chem>C2H3</chem>	=	1* <chem>C2H2</chem>	+	1* <chem>H</chem>	3.00000E+15	0.0000	32000.00
36	1* <chem>C2H3</chem>	+	1* <chem>O2</chem>	=	1* <chem>CH2O</chem>	+	1* <chem>HCO</chem>	3.98000E+12	0.0000	-250.00
37	1* <chem>C2H3</chem>	+	1* <chem>H</chem>	=	1* <chem>C2H2</chem>	+	1* <chem>H2</chem>	6.00000E+12	0.0000	0.00
38	1* <chem>C2H3</chem>	+	1* <chem>OH</chem>	=	1* <chem>C2H2</chem>	+	1* <chem>H2O</chem>	5.01200E+12	0.0000	0.00
39	1* <chem>C2H3</chem>	+	1* <chem>CH2</chem>	=	1* <chem>C2H2</chem>	+	1* <chem>CH3</chem>	3.02000E+13	0.0000	0.00
40	1* <chem>C2H3</chem>	+	1* <chem>C2H</chem>	=	2* <chem>C2H2</chem>	+		3.02000E+13	0.0000	0.00
41	1* <chem>C2H3</chem>	+	1* <chem>O</chem>	=	1* <chem>C2H2O</chem>	+	1* <chem>H</chem>	3.30000E+13	0.0000	0.00
42			2* <chem>CH2</chem>	=	1* <chem>C2H2</chem>	+	1* <chem>H2</chem>	4.00000E+13	0.0000	0.00
43			2* <chem>CH2</chem>	=	1* <chem>C2H3</chem>	+	1* <chem>H</chem>	5.01200E+12	0.0000	0.00
44	1* <chem>CH2</chem>	+	1* <chem>OH</chem>	=	1* <chem>CH</chem>	+	1* <chem>H2O</chem>	2.51000E+11	0.6700	25700.00
45	1* <chem>CH2</chem>	+	1* <chem>O</chem>	=	1* <chem>CH</chem>	+	1* <chem>OH</chem>	2.00000E+11	0.6800	25000.00
46	1* <chem>CH2</chem>	+	1* <chem>O2</chem>	=	1* <chem>CO2</chem>	+	2* <chem>H</chem>	1.59000E+12	0.0000	1000.00
47	M	+	1* <chem>C2H2</chem>	=	1* <chem>C2H</chem>	+	1* <chem>H</chem>	4.16900E+16	0.0000	107000.00
48			2* <chem>C2H2</chem>	=	1* <chem>C4H3</chem>	+	1* <chem>H</chem>	2.00000E+12	0.0000	45900.00
49	1* <chem>C2H2</chem>	+	1* <chem>O</chem>	=	1* <chem>CH2</chem>	+	1* <chem>CO</chem>	1.60000E+14	0.0000	9890.00
50	1* <chem>C2H2</chem>	+	1* <chem>O</chem>	=	1* <chem>C2HO</chem>	+	1* <chem>H</chem>	4.00000E+14	0.0000	10660.00
51	1* <chem>C2H2</chem>	+	1* <chem>OH</chem>	=	1* <chem>C2H</chem>	+	1* <chem>H2O</chem>	6.51000E+12	0.0000	7000.00

TABLE E.2.—Continued.

(i) Continued.

52	1*CH2	+	1*OH	=	1*CH2H2O	+	1*H	3.20000E+11	0.0000	200.00
53	1*CH2	+	1*CH2	=	1*CH4	+	1*H	3.00000E+13	0.0000	0.00
54	1*CH2	+	1*CH2	=	1*CH3	+	1*H	1.20000E+13	0.0000	6600.00
55	M	+	1*CH4	=	1*CH3	+	1*H	2.00000E+17	0.0000	65000.00
56	1*CH2H2O	+	1*OH	=	1*CH2O	+	1*HCO	2.80000E+13	0.0000	0.00
57	1*CH2H2O	+	1*OH	=	1*CH2O	+	1*H2O	7.50000E+12	0.0000	3000.00
58	1*CH2H2O	+	1*H	=	1*CH3	+	1*CO	1.13000E+13	0.0000	3428.00
59	1*CH2H2O	+	1*H	=	1*CH2H2O	+	1*H2	7.50000E+13	0.0000	8000.00
60	1*CH2H2O	+	1*O	=	1*CH2H2O	+	1*OH	5.00000E+13	0.0000	8000.00
61	1*CH2H2O	+	1*O	=	1*CH2H2O	+	1*CO	2.00000E+13	0.0000	0.00
62	M	+	1*CH2H2O	=	1*CH2	+	1*CO	2.00000E+16	0.0000	60000.00
63	1*CH2H2O	+	1*O2	=	2*CO	+	1*OH	1.46000E+12	0.0000	2500.00
64	1*CH2H2O	+	1*O	=	2*CO	+	1*H	1.20200E+12	0.0000	0.00
65	1*CH2H2O	+	1*OH	=	2*HCO	+	1*H	1.00000E+13	0.0000	0.00
66	1*CH2H2O	+	1*H	=	1*CH2	+	1*CO	5.00000E+13	0.0000	0.00
67	1*CH2H2O	+	1*CH2	=	1*CH2H3	+	1*CO	3.00000E+13	0.0000	0.00
68	1*CH2H2O	+	1*CH2	=	1*CH2O	+	1*CH2H	1.00000E+13	0.0000	2000.00
69			2*CH2H2O	=	1*CH2H2	+	2*CO	1.00000E+13	0.0000	0.00
70	1*CH2H	+	1*OH	=	1*CH2H2O	+	1*H	2.00000E+13	0.0000	0.00
71	1*CH2H	+	1*O2	=	1*CH2H2O	+	1*O	5.00000E+13	0.0000	1500.00
72	1*CH2H	+	1*O	=	1*CO	+	1*CH	5.01200E+13	0.0000	0.00
73	M	+	1*CH4	=	1*CH3	+	1*H	2.00000E+17	0.0000	88000.00
74	1*CH4	+	1*O2	=	1*CH3	+	1*H2O	7.94300E+13	0.0000	56000.00
75	1*CH4	+	1*H	=	1*CH3	+	1*H2	1.26000E+14	0.0000	11900.00
76	1*OH	+	1*CH4	=	1*CH3	+	1*H2O	2.50000E+13	0.0000	5010.00
77	1*O	+	1*CH4	=	1*CH3	+	1*OH	1.90000E+14	0.0000	11720.00
78	1*CH3	+	1*O2	=	1*CH3O	+	1*O	6.78600E+13	0.0000	29000.00
79	1*CH3	+	1*OH	=	1*CH3O	+	1*H	6.30000E+12	0.0000	0.00
80	M	+	1*CH3O	=	1*CH2O	+	1*H	5.00000E+13	0.0000	21000.00
81	1*CH3O	+	1*O2	=	1*CH2O	+	1*H2O	1.00000E+12	0.0000	6000.00
82	1*CH3O	+	1*H	=	1*CH2O	+	1*H2	2.00000E+13	0.0000	0.00
83			2*CH3	=	1*CH2H4	+	1*H2	1.00000E+16	0.0000	32000.00
84	1*CH3	+	1*O	=	1*CH2O	+	1*H	1.28800E+14	0.0000	2000.00
85	1*CH3	+	1*CH2O	=	1*CH4	+	1*HCO	1.00000E+10	0.0000	6000.00
86	1*CH3	+	1*HCO	=	1*CH4	+	1*CO	5.02000E+11	0.5000	0.00
87	1*CH3	+	1*H2O	=	1*CH3O	+	1*OH	2.00000E+13	0.0000	0.00
88	M	+	1*CH2O	=	1*HCO	+	1*H	5.00000E+16	0.0000	81000.00
89	1*CH2O	+	1*OH	=	1*HCO	+	1*H2O	3.00000E+13	0.0000	1200.00
90	1*CH2O	+	1*H	=	1*HCO	+	1*H2	2.50000E+13	0.0000	3990.00
91	1*CH2O	+	1*O	=	1*HCO	+	1*OH	3.50000E+13	0.0000	3510.00
92	1*HCO	+	1*H2O	=	1*CH2O	+	1*O2	1.00000E+14	0.0000	3000.00
93	M	+	1*HCO	=	1*H	+	1*CO	2.94000E+14	0.0000	15569.00
94	1*HCO	+	1*O2	=	1*CO	+	1*H2O	3.51100E+12	0.0000	7000.00
95	1*HCO	+	1*OH	=	1*CO	+	1*H2O	1.00000E+14	0.0000	0.00
96	1*HCO	+	1*H	=	1*CO	+	1*H2	1.99500E+14	0.0000	0.00
97	1*HCO	+	1*O	=	1*CO	+	1*OH	1.00000E+14	0.0000	0.00
98	1*CH	+	1*O2	=	1*HCO	+	1*O	1.00000E+13	0.0000	0.00
99	1*CO	+	1*O	=	1*CO2	+	M	5.90000E+15	0.0000	4100.00
100	1*CO	+	1*O2	=	1*CO2	+	1*O	2.50000E+12	0.0000	47690.00
101	1*CO	+	1*OH	=	1*CO2	+	1*H	4.17000E+11	0.0000	1000.00
102	1*CO	+	1*H2O	=	1*CO2	+	1*OH	5.75000E+13	0.0000	22930.00
103	1*O	+	1*H2O	=	2*OH	+	1*H	6.80000E+13	0.0000	18365.00
104	1*H	+	1*O2	=	1*OH	+	1*O	1.89000E+14	0.0000	16400.00
105	1*O	+	1*H2	=	1*OH	+	1*H	4.20000E+14	0.0000	13750.00
106	1*H	+	1*H2O	=	1*H2	+	1*O2	7.28000E+13	0.0000	2126.00
107	1*O	+	1*H2O	=	1*OH	+	1*O2	5.00000E+13	0.0000	1000.00
108	1*H2O	+	1*OH	=	1*H2O	+	1*O2	8.00000E+12	0.0000	0.00
109	1*H	+	1*H2O	=	2*OH	+	1*H	1.34000E+14	0.0000	1070.00
110	1*H2	+	1*H2O	=	1*H2O2	+	1*H	7.91000E+13	0.0000	25000.00
111	1*OH	+	1*H2O2	=	1*H2O	+	1*H2O2	6.10000E+12	0.0000	1430.00
112			2*H2O2	=	1*H2O2	+	1*O2	1.80000E+12	0.0000	0.00
113	1*H	+	1*H2O2	=	1*OH	+	1*H2O	7.80000E+11	0.0000	0.00
114	M	+	1*H2O2	=	2*OH	+	1*H	1.44000E+17	0.0000	45510.00
115	1*H2	+	1*OH	=	1*H2O	+	1*H	4.74000E+13	0.0000	6098.00
116	1*H	+	1*O2	=	1*H2O2	+	M	1.46000E+15	0.0000	-1000.00
117	M	+	1*H2O	=	1*H	+	1*OH	1.30000E+15	0.0000	105140.00
118	1*H	+	1*O	=	1*OH	+	M	7.10000E+18	-1.0000	0.00
119	M	+	1*H2	=	2*H	+		2.20000E+14	0.0000	96000.00
120	M	+	1*O2	=	2*O	+		1.80000E+18	-1.0000	118020.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(CH2	,114) = 2.30000	M(O2	,114) = 0.78000	M(CH2O	,114) = 6.00000	M(CH2O2	,114) = 6.60000
M(O2	,116) = 1.30000	M(CO2	,116) = 7.00000	M(CH2O	,116) = 21.30000	M(H2	,116) = 3.00000
M(C6H6	,116) = 20.00000	M(CH4	,116) = 5.00000	M(H2	,117) = 4.00000	M(O2	,117) = 1.50000
M(CH2O	,117) = 20.00000	M(C6H6	,117) = 20.00000	M(CO2	,117) = 4.00000	M(H2	,119) = 4.10000
M(O2	,119) = 2.00000	M(CH2O	,119) = 15.00000				

TABLE E.2.—Continued.
(i) Continued.

** INITIAL CONDITIONS **									
TIME	0.00000E+00	SEC	AREA	0.00000E+00	SQ CM	AXIAL POSITION	0.00000E+00	CM	
FLOW PROPERTIES					INTEGRATION INDICATORS				
PRESSURE (ATM)	2.38680		STEPS FROM LAST PRINT	0					
VELOCITY (CM/SEC)	0.00		AVERAGE STEP SIZE	0.00000E+00					
DENSITY (G/CM**3)	8.19683E-04		METHOD ORDER	0					
TEMPERATURE (DEG K)	1405.00		TOTAL NUMBER OF STEPS	0					
MASS FLOW RATE (G/SEC)	0.00000E+00		FUNCT EVALUATIONS	0					
ENTROPY (CAL/G/DEG K)	1.1945		JACOBIAN EVALUATIONS	0					
MACH NUMBER	0.0000								
GAMMA	1.4607								
ENTHALPY (CAL/G)	1.76459E+02								
SP. HEAT (CP) (CAL/G/DEG K)	1.59128E-01								
CHEMICAL PROPERTIES									
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE-CM**3/G**2/SEC)	NET RATE/POST-TIVE DIR RATE		
C6H6	3.49878E-07	1.69000E-02	-1.87557E-04	1	2.0574E+08	2.79071E+02	1.00000		
O2	2.60483E-06	1.25820E-01	-1.87502E-04	2	9.5467E+10	0.00000E+00	0.00000		
C6H5O	0.00000E+00	0.00000E+00	1.87502E-04	3	1.5865E-01	8.26167E-02	1.00000		
OH	0.00000E+00	0.00000E+00	1.87502E-04	4	8.1118E+11	0.00000E+00	0.00000		
C6H5	0.00000E+00	0.00000E+00	5.55085E-08	5	4.7946E+12	0.00000E+00	0.00000		
C12H10	0.00000E+00	0.00000E+00	0.00000E+00	6	4.1339E+12	0.00000E+00	0.00000		
H	0.00000E+00	0.00000E+00	5.55085E-08	7	4.6442E+06	0.00000E+00	0.00000		
H2	0.00000E+00	0.00000E+00	0.00000E+00	8	3.7236E+04	0.00000E+00	0.00000		
O	0.00000E+00	0.00000E+00	6.05693E-14	9	1.4463E+11	0.00000E+00	0.00000		
H2O	0.00000E+00	0.00000E+00	0.00000E+00	10	1.3979E+13	0.00000E+00	0.00000		
C4H3	0.00000E+00	0.00000E+00	0.00000E+00	11	2.3500E+02	0.00000E+00	0.00000		
C4H2	0.00000E+00	0.00000E+00	0.00000E+00	12	4.0973E+02	0.00000E+00	0.00000		
C5H5	0.00000E+00	0.00000E+00	0.00000E+00	13	1.2942E+12	0.00000E+00	0.00000		
CO	0.00000E+00	0.00000E+00	0.00000E+00	14	1.3523E+12	0.00000E+00	0.00000		
HO2	0.00000E+00	0.00000E+00	0.00000E+00	15	3.1799E+10	0.00000E+00	0.00000		
C2H2	0.00000E+00	0.00000E+00	0.00000E+00	16	1.9399E+03	0.00000E+00	0.00000		
C6H5OH	0.00000E+00	0.00000E+00	0.00000E+00	17	6.0009E+09	0.00000E+00	0.00000		
C5H6	0.00000E+00	0.00000E+00	0.00000E+00	18	3.0000E+13	0.00000E+00	0.00000		
C5H5O	0.00000E+00	0.00000E+00	0.00000E+00	19	1.7530E+13	0.00000E+00	0.00000		
H2O2	0.00000E+00	0.00000E+00	0.00000E+00	20	1.3927E+14	0.00000E+00	0.00000		
C4H5	0.00000E+00	0.00000E+00	0.00000E+00	21	1.0000E+13	0.00000E+00	0.00000		
C5H4OH	0.00000E+00	0.00000E+00	0.00000E+00	22	1.0000E+13	0.00000E+00	0.00000		
C6H4	0.00000E+00	0.00000E+00	0.00000E+00	23	3.7833E+11	0.00000E+00	0.00000		
HCN	0.00000E+00	0.00000E+00	0.00000E+00	24	2.0000E+13	0.00000E+00	0.00000		
C2H3	0.00000E+00	0.00000E+00	0.00000E+00	25	3.1000E+12	0.00000E+00	0.00000		

TABLE E.2.—Continued.

(i) Continued.

C2H0	0.00000E+00	0.00000E+00	0.00000E+00	26	1.0678E+04	0.00000E+00	0.00000
C2H	0.00000E+00	0.00000E+00	0.00000E+00	27	1.0000E+13	0.00000E+00	0.00000
C3H2	0.00000E+00	0.00000E+00	0.00000E+00	28	3.0000E+13	0.00000E+00	0.00000
C2H4	0.00000E+00	0.00000E+00	0.00000E+00	29	1.2000E+12	0.00000E+00	0.00000
CH3	0.00000E+00	0.00000E+00	0.00000E+00	30	9.1477E+04	0.00000E+00	0.00000
CH2O	0.00000E+00	0.00000E+00	0.00000E+00	31	3.0807E+12	0.00000E+00	0.00000
CH2	0.00000E+00	0.00000E+00	0.00000E+00	32	2.2090E+12	0.00000E+00	0.00000
C2H2O	0.00000E+00	0.00000E+00	0.00000E+00	33	4.1905E+12	0.00000E+00	0.00000
CH	0.00000E+00	0.00000E+00	0.00000E+00	34	1.4145E+12	0.00000E+00	0.00000
CO2	0.00000E+00	0.00000E+00	0.00000E+00	35	3.1585E+10	0.00000E+00	0.00000
C3H5	0.00000E+00	0.00000E+00	0.00000E+00	36	4.3528E+12	0.00000E+00	0.00000
C3H4	0.00000E+00	0.00000E+00	0.00000E+00	37	6.0000E+12	0.00000E+00	0.00000
CH4	0.00000E+00	0.00000E+00	0.00000E+00	38	5.0120E+12	0.00000E+00	0.00000
CH3O	0.00000E+00	0.00000E+00	0.00000E+00	39	3.0200E+13	0.00000E+00	0.00000
AR	1.77481E-05	8.57280E-01	0.00000E+00	40	3.0200E+13	0.00000E+00	0.00000
				41	3.3000E+13	0.00000E+00	0.00000
				42	4.0000E+13	0.00000E+00	0.00000
				43	5.0120E+12	0.00000E+00	0.00000
				44	3.2430E+09	0.00000E+00	0.00000
				45	3.5700E+09	0.00000E+00	0.00000
				46	1.1113E+12	0.00000E+00	0.00000
				47	9.4630E-01	0.00000E+00	0.00000
				48	1.4495E+05	0.00000E+00	0.00000
				49	4.6314E+12	0.00000E+00	0.00000
				50	8.7878E+12	0.00000E+00	0.00000
				51	5.1424E+11	0.00000E+00	0.00000
				52	2.9788E+11	0.00000E+00	0.00000
				53	3.0000E+13	0.00000E+00	0.00000
				54	1.1286E+12	0.00000E+00	0.00000
				55	1.5495E+07	0.00000E+00	0.00000
				56	2.8000E+13	0.00000E+00	0.00000
				57	2.5610E+12	0.00000E+00	0.00000
				58	3.3102E+12	0.00000E+00	0.00000
				59	4.2722E+12	0.00000E+00	0.00000
				60	2.8481E+12	0.00000E+00	0.00000
				61	2.0000E+13	0.00000E+00	0.00000
				62	9.2884E+06	0.00000E+00	0.00000
				63	5.9631E+11	0.00000E+00	0.00000
				64	1.2020E+12	0.00000E+00	0.00000
				65	1.0000E+13	0.00000E+00	0.00000
				66	5.0000E+13	0.00000E+00	0.00000
				67	3.0000E+13	0.00000E+00	0.00000
				68	4.8854E+12	0.00000E+00	0.00000
				69	1.0000E+13	0.00000E+00	0.00000
				70	2.0000E+13	0.00000E+00	0.00000
				71	2.9217E+13	0.00000E+00	0.00000
				72	5.0120E+13	0.00000E+00	0.00000
				73	4.0973E+03	0.00000E+00	0.00000
				74	1.5456E+05	0.00000E+00	0.00000
				75	1.7754E+12	0.00000E+00	0.00000
				76	4.1555E+12	0.00000E+00	0.00000
				77	2.8556E+12	0.00000E+00	0.00000
				78	1.4756E+09	0.00000E+00	0.00000
				79	6.3000E+12	0.00000E+00	0.00000
				80	2.7064E+10	0.00000E+00	0.00000
				81	1.1660E+11	0.00000E+00	0.00000
				82	2.0000E+13	0.00000E+00	0.00000
				83	1.0528E+11	0.00000E+00	0.00000
				84	6.2924E+13	0.00000E+00	0.00000
				85	4.3705E+10	0.00000E+00	0.00000
				86	1.1320E+13	0.00000E+00	0.00000
				87	2.0000E+13	0.00000E+00	0.00000
				88	1.2569E+04	0.00000E+00	0.00000
				89	1.9519E+13	0.00000E+00	0.00000
				90	5.9881E+12	0.00000E+00	0.00000
				91	9.9559E+12	0.00000E+00	0.00000
				92	3.4166E+13	0.00000E+00	0.00000
				93	1.1132E+12	0.00000E+00	0.00000
				94	2.6984E+11	0.00000E+00	0.00000
				95	1.0000E+14	0.00000E+00	0.00000
				96	1.9950E+14	0.00000E+00	0.00000
				97	1.0000E+14	0.00000E+00	0.00000
				98	1.0000E+13	0.00000E+00	0.00000
				99	1.3586E+15	0.00000E+00	0.00000
				100	9.5431E+04	0.00000E+00	0.00000
				101	2.9166E+11	0.00000E+00	0.00000
				102	1.5591E+10	0.00000E+00	0.00000
				103	9.4582E+10	0.00000E+00	0.00000
				104	5.3140E+11	0.00000E+00	0.00000
				105	3.0508E+12	0.00000E+00	0.00000
				106	3.3996E+13	0.00000E+00	0.00000
				107	3.4948E+13	0.00000E+00	0.00000
				108	8.0000E+12	0.00000E+00	0.00000
				109	9.1341E+13	0.00000E+00	0.00000
				110	1.0219E+10	0.00000E+00	0.00000
				111	3.6550E+12	0.00000E+00	0.00000
				112	1.8000E+12	0.00000E+00	0.00000
				113	7.8000E+11	0.00000E+00	0.00000
				114	1.2001E+10	0.00000E+00	0.00000
				115	5.3361E+12	0.00000E+00	0.00000
				116	2.0888E+15	0.00000E+00	0.00000
				117	5.7447E-02	0.00000E+00	0.00000
				118	5.0534E+15	0.00000E+00	0.00000
				119	2.5673E-01	0.00000E+00	0.00000
				120	5.6158E-04	4.50745E-08	1.00000

DERIVATIVES (CGS UNITS): T -5.10692E+03 RHO 0.00000E+00
MIXTURE MOLECULAR WEIGHT 39.59283 TOTAL ENERGY EXCHANGE RATE 2.68773E+05 MASS FRACTION SUM 1.00000000
(CAL-CM**3/G**2/SEC)

CPU TIME FOR INITIALIZATION OF LSENS = 2.129997 S

TABLE E.2.—Continued.

(i) Continued.

TIME	5.02811E-04	SEC	AREA	0.00000E+00	SQ CM	AXIAL POSITION	0.00000E+00	CM
FLOW PROPERTIES					INTEGRATION INDICATORS			
PRESSURE (ATM)	5.63501		STEPS FROM LAST PRINT	50				
VELOCITY (CM/SEC)	0.00		AVERAGE STEP SIZE	0.81053E-06				
DENSITY (G/CM**3)	8.19683E-04		METHOD ORDER	5				
TEMPERATURE (DEG K)	2068.59							
MASS FLOW RATE (G/SEC)	0.00000E+00		TOTAL NUMBER OF STEPS	200				
ENTROPY (CAL/G/DEG K)	1.2812		FUNCT EVALUATIONS	505				
MACH NUMBER	0.0000		JACOBIAN EVALUATIONS	56				
GAMMA	1.4813							
ENTHALPY (CAL/G)	2.13338E+02							
SP. HEAT (CP) (CAL/G/DEG K)	1.59794E-01							
CHEMICAL PROPERTIES								
SPECIES	CONCENTRATION (MOLES/CM**3)	MOLE FRACTION	NET SPECIES PRODUCTION RATE (MOLE/CM**3/SEC)	REACTION NUMBER	RATE CONST CGS UNITS	NET REACTION CONV RATE (MOLE/CM**3/SEC)	NET RATE/POSITIVE DIR RATE	
C6H6	1.95706E-08	9.13868E-04	-1.16032E-02	1	1.0E+11	4.98496E+02	0.99958	
O2	1.67548E-06	7.81449E-02	-1.40865E-01	2	1.5117E+11	5.82333E+02	0.97421	
C6H5O	3.77703E-09	1.76372E-04	-1.37938E-03	3	3.8E+10	-1.09910E+04	0.90660	
C6H5	6.27176E-08	2.92865E-03	3.07656E-02	4	5.0994E+12	3.60007E+03	0.98308	
C6H5	5.50165E-09	1.63513E-04	-1.30945E-03	5	8.4E+12	1.20854E+04	0.99848	
C12H10	4.41770E-09	2.06289E-04	-4.90881E-04	6	6.9E+12	1.25907E+04	0.98502	
H	2.46542E-08	1.15125E-03	1.20295E-02	7	4.5805E+09	1.04350E+03	0.99899	
H2	2.52278E-08	1.17804E-03	4.91811E-03	8	5.7753E+06	3.24665E+04	1.00000	
O	4.92998E-08	2.30210E-03	2.83327E-02	9	3.4E+11	2.89061E+03	0.97157	
H2O	4.92184E-07	2.29830E-02	4.89969E-02	10	1.5681E+13	4.03808E+01	0.99929	
C4H2	7.15660E-09	3.34091E-04	1.77918E-03	11	9.7E+10	5.09571E+03	0.99996	
C5H5	3.16265E-08	1.47683E-03	-1.03612E-02	12	1.0E+10	-3.54713E+04	0.12375	
CO	9.92200E-07	4.63318E-02	1.11641E-01	13	3.2E+12	6.84638E+01	0.03356	
H2O2	4.94453E-10	2.30890E-05	-4.81231E-05	14	5.6E+12	3.44714E+03	0.99820	
C2H2	2.03958E-08	9.52311E-04	-7.68259E-03	15	5.7E+11	-1.12432E+02	0.19851	
C6H5OH	1.67321E-08	7.81323E-04	-9.96410E-03	16	5.1E+10	5.19566E+03	0.08509	
C5H6	7.93748E-09	3.70649E-04	-4.42616E-03	17	6.4E+10	1.28162E+03	1.00000	
C5H5O	2.16902E-17	1.01284E-12	3.29176E-07	18	3.0E+03	4.67815E+04	0.99840	
H2O2	1.13976E-11	5.32223E-07	1.00283E-06	19	2.0E+13	2.53738E+02	0.98957	
C4H5	3.58781E-12	1.67536E-07	-1.77523E-06	20	7.8E+14	2.49529E+04	0.99057	
C5H6OH	7.07076E-15	3.30176E-10	-3.12696E-07	21	1.0E+00	2.52062E+04	1.00000	
C4H4	9.27112E-08	4.32924E-03	1.98356E-02	22	1.0E+00	2.95221E+04	1.00000	
HCO	2.71147E-10	1.26615E-05	2.06916E-05	23	4.7E+12	2.95225E+04	0.59198	
C2H3	5.31954E-10	2.48401E-05	3.56206E-06	24	2.0E+00	4.65495E+02	1.00000	
C2H10	8.48947E-09	3.96424E-04	6.98143E-04	25	3.1E+12	-1.48276E+02	0.72383	
C2H	3.21662E-11	1.50110E-06	1.12092E-05	26	4.6E+10	2.49555E+04	0.99869	
C3H2	6.91686E-10	3.22990E-05	4.52965E-04	27	1.0E+00	1.71351E+02	0.99970	
C2H4	4.51217E-12	2.10700E-07	-5.34455E-07	28	3.0E+00	6.53612E+02	0.99938	
CH3	5.07427E-11	2.36948E-06	-5.01826E-06	29	1.2E+12	2.05640E+01	1.00000	
CH2O	2.67723E-09	1.25016E-04	-1.05448E-03	30	6.5E+10	8.60995E-02	0.91959	
CH2	7.02250E-09	3.27923E-04	2.79024E-03	31	3.5E+12	-2.18709E+00	0.59406	
C2H2O	6.55580E-10	3.06130E-05	-3.48518E-05	32	2.5E+12	8.32743E-01	1.00000	
CH	8.02821E-12	3.74885E-07	8.95177E-06	33	7.4E+12	1.41809E+00	0.57544	
CO2	1.16338E-07	5.43252E-03	3.69010E-02	34	1.5E+12	6.61516E-01	0.99435	
C3H3	1.41642E-09	6.61411E-05	2.48428E-04	35	1.2E+12	2.05146E+04	0.97110	
C3H4	4.73461E-10	2.21087E-05	7.81681E-05	36	4.2E+12	5.60402E+03	1.00000	
CH3O	5.71018E-12	2.66643E-07	-9.54263E-07	37	6.0E+12	1.17113E+02	0.99995	
CH3O	1.40651E-13	6.56784E-09	-4.75547E-09	38	5.0E+12	2.48865E+02	0.99996	
AR	1.77481E-05	8.28766E-01	0.00000E+00	39	3.0E+00	1.67912E+02	1.00000	
				40	3.0E+00	7.67487E-01	0.99851	
				41	3.3E+00	1.28808E+03	1.00000	
				42	4.0E+00	2.93597E+03	1.00000	
				43	5.0E+12	3.67877E+02	1.00000	
				44	8.0E+10	5.27685E+01	0.99966	
				45	8.2E+10	4.22963E+01	0.99966	
				46	1.2E+12	2.18055E+04	1.00000	
				47	2.0E+10	-2.46745E+00	0.94836	
				48	2.8E+00	-1.40501E+03	0.99999	
				49	1.4E+12	2.15912E+04	0.99999	
				50	2.9E+10	4.47018E+04	0.99875	
				51	1.1E+12	2.12881E+03	0.97291	
				52	3.0E+11	5.79690E+02	0.99904	
				53	3.0E+00	-9.30694E+01	0.76073	
				54	2.4E+12	4.86093E+02	0.94654	
				55	2.7E+12	-1.16342E+02	0.22119	
				56	2.8E+00	1.71317E+03	0.99982	
				57	3.6E+12	-6.91095E+01	0.23804	
				58	4.9E+12	1.18059E+02	0.99993	
				59	1.0E+11	-1.24257E+02	0.32534	
				60	7.1E+12	-1.01311E+02	0.22776	
				61	2.0E+00	9.62074E+02	1.00000	
				62	9.1E+10	-5.78988E+02	0.75153	
				63	7.9E+11	1.68048E+04	1.00000	
				64	1.2E+12	7.48752E+02	1.00000	
				65	1.0E+00	7.92459E+03	1.00000	
				66	5.0E+00	1.55090E+04	0.99571	
				67	3.0E+00	2.66196E+03	1.00000	
				68	6.1E+12	5.45476E+02	1.00000	
				69	1.0E+00	1.07268E+03	1.00000	
				70	2.0E+00	5.72112E+01	0.95329	
				71	5.4E+13	2.74332E+03	0.98702	
				72	5.0E+12	1.18221E+02	1.00000	
				73	1.0E+10	-4.65289E+00	0.99607	
				74	9.6E+12	-1.80108E-02	0.92935	
				75	6.9E+12	8.73049E-01	0.59796	
				76	7.3E+12	2.53672E+00	0.64402	
				77	1.0E+12	2.98404E+00	0.64876	
				78	4.1E+10	3.63130E+00	0.69547	
				79	6.1E+12	-2.85430E+00	0.08730	
				80	5.2E+11	1.36073E+00	0.98964	
				81	2.2E+11	8.13418E-02	0.99542	
				82	2.0E+00	1.03220E-01	0.99998	
				83	4.1E+12	1.58959E-02	0.99683	
				84	7.1E+10	2.94804E+02	0.99998	
				85	1.5E+11	2.13530E-02	0.99945	
				86	1.7E+12	2.81270E-01	0.99998	
				87	2.0E+00	7.41212E-01	0.99244	

TABLE E.2.—Continued.

(i) Continued.

88	1.5842E+08	1.01607E+01	0.86021
89	2.2405E+13	5.59804E+03	0.99980
90	9.4709E+12	9.30207E+02	0.99978
91	1.4902E+13	2.92676E+03	0.99981
92	4.8200E+13	-1.22740E+03	0.99222
93	6.6598E+12	5.72921E+04	0.99541
94	6.0311E+11	4.07214E+02	0.99974
95	1.0000E+14	2.53104E+03	0.99999
96	1.9950E+14	1.98492E+03	0.99999
97	1.0000E+14	1.98955E+03	0.99999
98	1.0000E+13	1.99962E+02	0.99999
99	2.1761E+15	3.39264E+03	1.00000
100	2.2878E+07	5.61387E+01	0.99996
101	5.2695E+11	2.95091E+04	0.99291
102	2.1731E+11	1.58649E+02	0.97449
103	7.8023E+11	3.75030E+02	0.99982
104	3.4977E+12	1.55084E+05	0.01331
105	1.4810E+13	3.46399E+05	0.72205
106	4.3403E+13	7.65113E+02	0.12636
107	3.9203E+13	1.38702E+05	0.97159
108	8.0000E+12	5.59955E+02	0.97518
109	1.0329E+14	1.86113E+03	0.97485
110	1.8067E+11	-1.64242E+01	0.99310
111	4.3077E+12	3.89488E+00	0.83041
112	1.8000E+12	5.45280E-01	0.84984
113	7.8000E+11	3.25880E-01	0.83251
114	2.2396E+12	2.32146E+02	0.99896
115	1.0753E+13	2.90117E+03	0.25957
116	1.8621E+15	3.56669E+03	0.11457
117	1.0133E+04	-1.71692E+02	0.94438
118	3.4323E+15	1.32785E+02	0.99860
119	1.5845E+04	-1.13010E+01	0.99862
120	2.9554E+02	-3.15872E+00	0.99842
120			0.99503

DERIVATIVES (CGS UNITS): T 7.54742E+07 RHO 0.00000E+00
MIXTURE MOLECULAR WEIGHT 38.27592 TOTAL ENERGY EXCHANGE RATE -8.88370E+09 MASS FRACTION SUM 1.00000002
(CAL-CM**3/G**2/SEC)

COMPUTER TIME (CPU) REQUIRED: FOR THIS STEP - 2.054000E+01 S UP TO THIS TIME - 8.349001E+01 S

***** SENSITIVITY CALCULATIONS *****

TIME = 3.02811D-04

SENSITIVITY COEFFICIENTS OF 0-ORDER TIME DERIVATIVE OF DEPENDENT VARIABLES

**** SENSITIVITY TO INITIAL CONDITIONS ****

DZ(I)/DYZERO(J)*F(J)/Z(I), WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW
F(J)= YZERO(J) FOR YZERO(J) NOT EQUAL TO 0
= 1.0E-4/(INITIAL MWT) FOR YZERO(J) = 0

PARAMETER	C6H6	C6H5	H2O	CO	C2H2	C6H5OH	C5H6	TEMP	PRESSURE
C6H6	-4.595D+01	-2.848D+01	8.699D+00	9.844D+00	-2.875D+01	-4.749D+01	-4.410D+01	3.063D+00	3.524D+00
OH	-6.884D+00	-4.338D+00	1.157D+00	1.306D+00	-4.376D+00	-6.901D+00	-6.474D+00	4.239D-01	4.838D-01
AK	6.824D+01	4.281D+01	-1.129D+01	-1.290D+01	4.337D+01	6.916D+01	6.481D+01	-4.301D+00	-4.069D+00
TEMP	-2.049D+03	-1.291D+03	3.432D+02	3.882D+02	-1.303D+03	-2.056D+03	-1.928D+03	1.264D+02	1.442D+02
DENSITY	-1.173D+02	-7.382D+01	1.972D+01	2.223D+01	-7.451D+01	-1.171D+02	-1.103D+02	7.238D+00	9.254D+00

TABLE E.2.—Concluded.

(i) Concluded.

**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE PREEXPONENTIAL CONSTANTS ****

DZ(I)/DA(J)*A(J)/Z(I) WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

REAC NUM	C6H6	C6H5	H2O	CO	C2H2	C6H5OH	C5H6	TEMP	PRESSURE
1	-5.692D+01	-3.593D+01	9.534D+00	1.078D+01	-3.610D+01	-5.691D+01	-5.337D+01	3.494D+00	3.988D+00
2	2.059D+00	1.345D+00	-3.488D-01	-4.016D-01	1.283D+00	2.045D+00	1.904D+00	-1.283D-01	-1.466D-01
3	1.759D+00	5.978D-01	-2.539D-01	-2.868D-01	9.145D-01	1.413D+00	1.327D+00	-9.098D-02	-1.042D-01
4	-7.968D-01	-3.372D-01	1.145D-01	1.345D-01	-4.102D-01	-7.069D-01	-6.318D-01	4.205D-02	4.824D-02
5	1.277D+01	7.873D+00	-2.256D+00	-2.527D+00	8.691D+00	1.368D+01	1.290D+01	-8.285D-01	-9.445D-01
6	-2.174D+01	-1.315D+01	3.600D+00	4.073D+00	-1.337D+01	-2.139D+01	-1.989D+01	1.316D+00	1.502D+00
7	-1.162D-02	-8.334D-03	2.378D-03	3.055D-03	-1.203D-02	-5.860D-03	-8.083D-03	8.672D-04	1.010D-03
8	-6.044D-01	-3.803D-01	1.015D-01	1.150D-01	-3.853D-01	-6.101D-01	-5.643D-01	3.722D+00	4.249D+00
10	2.765D-01	1.708D-01	-4.691D-02	-5.283D-02	1.771D-01	2.811D-01	2.641D-01	-1.720D-02	-1.962D-02
11	1.364D-01	-1.754D-01	-3.387D-02	-4.276D-02	2.247D-01	2.255D-01	2.246D-01	-1.524D-02	-1.692D-02
12	4.142D+01	2.609D+01	-6.954D+00	-7.862D+00	2.635D+01	4.157D+01	3.890D+01	-2.551D+00	-2.911D+00
13	1.500D+00	9.419D-01	-2.518D-01	-2.830D-01	9.628D-01	1.513D+00	1.424D+00	-9.217D-02	-1.051D-01
14	7.860D-01	5.001D-01	-1.329D-01	-1.462D-01	5.060D-01	7.250D-01	7.140D-01	-4.803D-02	-5.471D-02
15	2.395D+00	1.508D+00	-4.029D-01	-4.553D-01	1.523D+00	2.404D+00	2.253D+00	-1.478D-01	-1.687D-01
16	-1.962D+01	-1.235D+01	3.306D+00	3.733D+00	-1.248D+01	-1.971D+01	-1.857D+01	1.213D+00	1.384D+00
17	-3.337D+01	-2.097D+01	5.645D+00	6.378D+00	-2.122D+01	-3.367D+01	-3.168D+01	2.071D+00	2.363D+00
18	1.903D+01	1.203D+01	-0.933D+00	-3.509D+00	1.218D+01	1.799D+01	1.738D+01	-1.142D+00	-1.303D+00
19	2.322D+00	1.459D+00	-3.969D-01	-4.502D-01	1.473D+00	2.352D+00	2.207D+00	-1.464D-01	-1.670D-01
20	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
21	-6.941D+00	-4.292D+00	1.251D+00	1.428D+00	-3.922D+00	-7.355D+00	-7.247D+00	4.655D-01	5.305D-01
101	-1.206D+00	-8.037D-01	1.901D-01	1.869D-01	-7.953D-01	-1.162D+00	-1.120D+00	8.560D-02	9.564D-02
104	-2.728D+01	-1.694D+01	4.551D+00	5.117D+00	-1.734D+01	-2.693D+01	-2.555D+01	1.656D+00	1.890D+00
116	-2.016D+00	-1.259D+00	3.413D-01	3.846D-01	-1.266D+00	-2.070D+00	-1.938D+00	1.251D-01	1.427D-01

**** NORMALIZED SENSITIVITY COEFFICIENTS W.R.T THE ACTIVATION ENERGIES ****

DZ(I)/DE(J)*E(J)/Z(I), WHERE Z(I)= 0-ORDER TIME DERIV. OF Y(I), I=COLUMN, J=ROW

REAC NUM	C6H6	C6H5	H2O	CO	C2H2	C6H5OH	C5H6	TEMP	PRESSURE
1	-5.600D+01	-3.534D+01	9.382D+00	1.061D+01	-3.553D+01	-5.601D+01	-5.252D+01	3.439D+00	3.925D+00
2	2.026D+00	1.315D+00	-3.443D-01	-3.963D-01	1.265D+00	2.019D+00	1.881D+00	-1.266D-01	-1.447D-01
3	1.517D+00	6.089D-01	-2.249D-01	-2.543D-01	8.174D-01	1.269D+00	1.189D+00	-8.098D-02	-9.270D-02
4	-7.708D-01	-3.742D-01	1.152D-01	1.341D-01	-4.206D-01	-7.035D-01	-6.374D-01	4.233D-02	4.850D-02
5	1.200D+01	7.427D+00	-2.095D+00	-2.350D+00	8.043D+00	1.266D+01	1.193D+01	-7.693D-01	-8.771D-01
6	-2.062D+01	-1.263D+01	3.425D+00	3.876D+00	-1.277D+01	-2.136D+01	-1.897D+01	1.235D+00	1.430D+00
7	-9.325D-03	-6.572D-03	1.876D-03	2.380D-03	-9.249D-03	-5.820D-03	-6.823D-03	6.852D-04	7.957D-04
8	-5.752D+01	-3.620D+01	9.658D+00	1.094D+01	-3.665D+01	-5.796D+01	-5.382D+01	3.543D+00	4.044D+00
10	2.589D-01	1.607D-01	-4.382D-02	-4.938D-02	1.655D-01	2.424D-01	2.465D-01	-1.607D-02	-1.833D-02
11	1.394D-01	-9.194D-02	-3.102D-02	-3.853D-02	1.857D-01	2.422D-01	1.980D-01	-1.345D-02	-1.499D-02
12	3.966D+01	2.498D+01	-6.659D+00	-7.527D+00	2.523D+01	3.979D+01	3.726D+01	-2.442D+00	-2.787D+00
13	1.497D+00	9.403D-01	-2.512D-01	-2.824D-01	9.596D-01	1.508D+00	1.419D+00	-9.193D-02	-1.049D-01
14	6.766D-01	4.302D-01	-1.142D-01	-1.261D-01	4.331D-01	6.332D-01	6.167D-01	-4.135D-02	-4.711D-02
15	2.290D+00	1.442D+00	-3.852D-01	-4.353D-01	1.456D+00	2.299D+00	2.155D+00	-1.413D-01	-1.613D-01
16	-1.901D+01	-1.197D+01	3.202D+00	3.618D+00	-1.209D+01	-1.409D+01	-1.797D+01	1.175D+00	1.341D+00
17	-3.128D+01	-1.967D+01	5.286D+00	5.973D+00	-1.990D+01	-3.333D+01	-2.966D+01	1.940D+00	2.213D+00
18	1.736D+01	1.098D+01	-2.836D+00	-3.213D+00	1.107D+01	1.459D+01	1.591D+01	-1.045D+00	-1.192D+00
19	2.121D+00	1.332D+00	-3.620D-01	-4.105D-01	1.345D+00	2.147D+00	2.013D+00	-1.335D-01	-1.522D-01
20	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00	0.000D+00
21	-6.596D+00	-4.092D+00	1.172D+00	1.335D+00	-3.860D+00	-6.916D+00	-6.737D+00	4.349D-01	4.958D-01
101	-1.035D+00	-6.820D-01	1.647D-01	1.651D-01	-6.770D-01	-1.007D+00	-9.656D-01	7.220D-02	8.086D-02
104	-2.491D+01	-1.553D+01	4.158D+00	4.680D+00	-1.582D+01	-2.465D+01	-2.333D+01	1.515D+00	1.730D+00
116	-1.955D+00	-1.224D+00	3.305D-01	3.726D-01	-1.233D+00	-1.496D+00	-1.871D+00	1.212D-01	1.382D-01

(LSNS) END OF THIS CASE

SUMMARY OF COMPUTATIONAL WORK REQUIRED FOR PROBLEM:

TOTAL NO. OF STEPS - 247
TOTAL NO. OF DERIVATIVE EVALUATIONS - 385
TOTAL NO. OF JACOBIAN EVALUATIONS - 44
TOTAL CPU TIME - 103.384999 S

WORK REQUIRED BY SENSITIVITY ROUTINE:

NO. STEPS = 247
NO. FUNC. EVAL. = 247
NO. JAC. EVAL. = 247
TOTAL REAL SPACE USED = 16824
TOTAL INTEGER SPACE USED = 124

TOTAL CPU TIME (INCLUDING I/O) REQUIRED = 108.609993 S

(LSNS) READ DATA FOR NEXT CASE

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REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188	
Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.				
1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE March 1994		3. REPORT TYPE AND DATES COVERED Reference Publication
4. TITLE AND SUBTITLE LSENS, A General Chemical Kinetics and Sensitivity Analysis Code for Homogeneous Gas-Phase Reactions III. Illustrative Test Problems			5. FUNDING NUMBERS WU-505-62-52	
6. AUTHOR(S) David A. Bittker and Krishnan Radhakrishnan				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) National Aeronautics and Space Administration Lewis Research Center Cleveland, Ohio 44135-3191			8. PERFORMING ORGANIZATION REPORT NUMBER E-5140-3	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) National Aeronautics and Space Administration Washington, D.C. 20546-0001			10. SPONSORING/MONITORING AGENCY REPORT NUMBER NASA RP-1330	
11. SUPPLEMENTARY NOTES David A. Bittker, NASA Lewis Research Center; and Krishnan Radhakrishnan, NYMA, Inc., Lewis Research Center Group, 2001 Aerospace Parkway, Brook Park, Ohio 44142. Responsible person, Edward J. Mularz, organization code 2650, (216) 433-5850.				
12a. DISTRIBUTION/AVAILABILITY STATEMENT Unclassified - Unlimited Subject Categories 25 and 64			12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words) LSENS, the Lewis General Chemical Kinetics and Sensitivity Analysis Code, has been developed for solving complex, homogeneous, gas-phase chemical kinetics problems and contains sensitivity analysis for a variety of problems, including nonisothermal situations. This report is part III of a series of three reference publications that describe LSENS, provide a detailed guide to its usage, and present many example problems. Part III explains the kinetics and kinetics-plus-sensitivity-analysis problems supplied with LSENS and presents sample results. These problems illustrate the various capabilities of, and reaction models that can be solved by, the code and may provide a convenient starting point for the user to construct the problem data file required to execute LSENS. LSENS is a flexible, convenient, accurate, and efficient solver for chemical reaction problems such as static system; steady, one-dimensional, inviscid flow; reaction behind incident shock wave, including boundary layer correction; and perfectly stirred (highly backmixed) reactor. In addition, the chemical equilibrium state can be computed for the following assigned states: temperature and pressure, enthalpy and pressure, temperature and volume, and internal energy and volume. For static problems the code computes the sensitivity coefficients of the dependent variables and their temporal derivatives with respect to the initial values of the dependent variables and/or the three rate coefficient parameters of the chemical reactions. Part I (NASA RP-1328) derives the governing equations and describes the numerical solution procedures for the types of problems that can be solved by LSENS. Part II (NASA RP-1329) describes LSENS, its usage, illustrated by example problems, and how to modify it.				
14. SUBJECT TERMS Chemical kinetics computation; Sensitivity analysis; Gas-phase chemical kinetics			15. NUMBER OF PAGES 152	
			16. PRICE CODE A08	
17. SECURITY CLASSIFICATION OF REPORT Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT Unclassified	20. LIMITATION OF ABSTRACT	